Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1204bxd

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS	4	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAplus
NEWS	5	FEB 05	German (DE) application and patent publication number format changes
NEWS	6	MAR 03	MEDLINE and LMEDLINE reloaded
NEWS	7	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	8	MAR 03	FRANCEPAT now available on STN
NEWS	9	MAR 29	Pharmaceutical Substances (PS) now available on STN
NEWS	10	MAR 29	WPIFV now available on STN
NEWS	11	MAR 29	No connect hour charges in WPIFV until May 1, 2004
NEWS	12	MAR 29	New monthly current-awareness alert (SDI) frequency in RAPRA
NEWS	13	APR 26	PROMT: New display field available
NEWS	14	APR 26	IFIPAT/IFIUDB/IFICDB: New super search and display field available
NEWS	15	APR 26	LITALERT now available on STN
NEWS	16	APR 27	NLDB: New search and display fields available

NEWS EXPRESS	MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:34:23 ON 05 MAY 2004

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.52	2.52

FILE 'REGISTRY' ENTERED AT 16:41:25 ON 05 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 MAY 2004 HIGHEST RN 679784-15-7
DICTIONARY FILE UPDATES: 4 MAY 2004 HIGHEST RN 679784-15-7

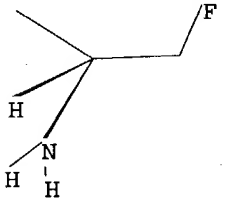
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

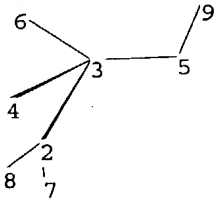
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\09857465.str





chain nodes :
2 3 4 5 6 7 8 9
chain bonds :
2-3 2-7 2-8 3-4 3-5 3-6 5-9
exact/norm bonds :
2-3
exact bonds :
2-7 2-8 3-4 3-5 3-6 5-9

G1:H,F

Match level :
2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

Stereo Bonds:

3-2 (Single Wedge).
4-3 (Single Hash).

Stereo Chiral Centers:

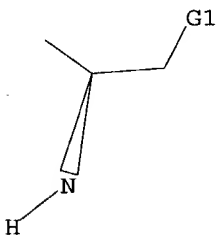
3 (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 3

L1 STRUCTURE UPLOADED

=> d query
L1 STR



G1 H,F

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 16:41:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 149342 TO ITERATE

0.7% PROCESSED 1000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 1000000

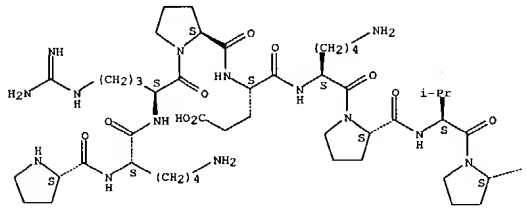
L2 50 SEA SSS SAM L1

=> d scan

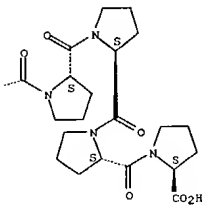
L2 50 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN L-Proline, L-prolyl-L-lysyl-L-arginyl-L-prolyl-L-α-glutamyl-L-lysyl-L-prolyl-L-valyl-L-prolyl-L-prolyl-L-prolyl-L-prolyl- (9CI)
SQL 13
MF C68 H110 N18 O16

Absolute stereochemistry.

PAGE 1-A



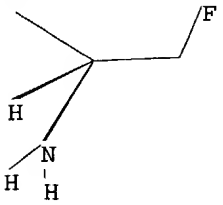
PAGE 1-B

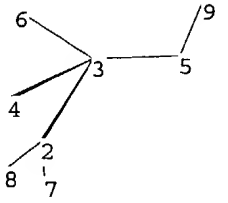


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>
Uploading C:\Program Files\Stnexp\Queries\09857465.str





chain nodes :
2 3 4 5 6 7 8 9
chain bonds :
2-3 2-7 2-8 3-4 3-5 3-6 5-9
exact/norm bonds :
2-3
exact bonds :
2-7 2-8 3-4 3-5 3-6 5-9

G1:H,F

Match level :
2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

Stereo Bonds:

3-2 (Single Wedge).
4-3 (Single Hash).

Stereo Chiral Centers:

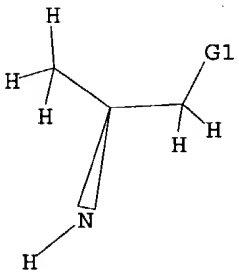
3 (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 3

L3 STRUCTURE UPLOADED

=> d query
L3 STR



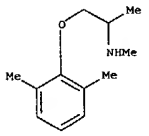
G1 H,F

Structure attributes must be viewed using STN Express query preparation.

```
=> s l3
SAMPLE SEARCH INITIATED 16:42:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 149342 TO ITERATE

  0.7% PROCESSED    1000 ITERATIONS                                 6 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS   16126

L4             6 SEA SSS SAM L3

=> d scan
```

L4 6 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Propanamine, 1-(2,6-dimethylphenoxy)-N-methyl-, (-)- (9CI)
MF C12 H19 N O
CI COM

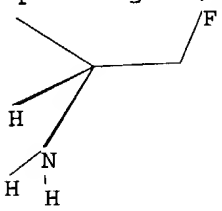
Rotation (-).

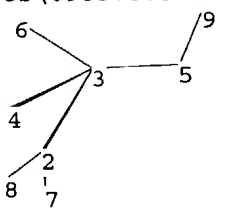


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>
Uploading C:\Program Files\Stnexp\Queries\09857465.str





chain nodes :
2 3 4 5 6 7 8 9
chain bonds :
2-3 2-7 2-8 3-4 3-5 3-6 5-9
exact/norm bonds :
2-3
exact bonds :
2-7 2-8 3-4 3-5 3-6 5-9

G1:H,F

Match level :
2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

Stereo Bonds:

3-2 (Single Wedge).
4-3 (Single Hash).

Stereo Chiral Centers:

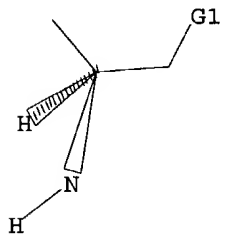
3 (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 3

L5 STRUCTURE UPLOADED

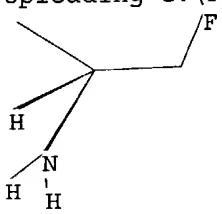
=> d query
L5 STR

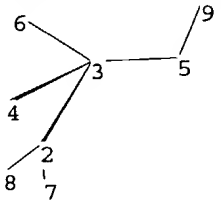


G1 H,F

Structure attributes must be viewed using STN Express query preparation.

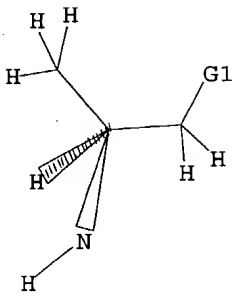
```
=> s l5
SAMPLE SEARCH INITIATED 16:46:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 149342 TO ITERATE

  0.7% PROCESSED    1000 ITERATIONS                                  50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS 1000000

L6            50 SEA SSS SAM L5

=>
Uploading C:\Program Files\Stnexp\Queries\09857465.str
```






```
chain nodes :
2  3  4  5  6  7  8  9
chain bonds :
2-3  2-7  2-8  3-4  3-5  3-6  5-9
exact/norm bonds :
2-3
exact bonds :
2-7  2-8  3-4  3-5  3-6  5-9


G1:H,F

Match level :
2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:CLASS  9:CLASS

Stereo Bonds:

3-2 (Single Wedge).
4-3 (Single Hash).


Stereo Chiral Centers:

3    (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 3

L7      STRUCTURE UPLOADED

=> d query
```

L7 STR



G1 H,F

Structure attributes must be viewed using STN Express query preparation.

=> s l7
SAMPLE SEARCH INITIATED 16:47:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 149342 TO ITERATE

0.7% PROCESSED 1000 ITERATIONS 4 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 10481

L8 4 SEA SSS SAM L7

=> s l7
SAMPLE SEARCH INITIATED 16:47:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 149342 TO ITERATE

0.7% PROCESSED 1000 ITERATIONS 4 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 10481

L9 4 SEA SSS SAM L7

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 4.20 6.72

FILE 'CAPLUS' ENTERED AT 16:47:42 ON 05 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

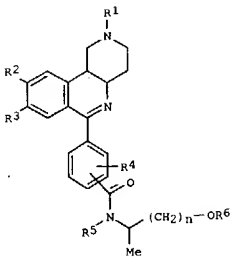
FILE COVERS 1907 - 5 May 2004 VOL 140 ISS 19
FILE LAST UPDATED: 4 May 2004 (20040504/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

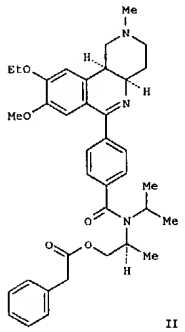
=> s l9
L10 6 L9

=> d l10 1-6 abs ibib hitstr

L10 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I



II

AB The title compds. I [R1 = C1-C4 alkyl; R2, R3 = OH, C1-C4 alkoxy, C3-C7 cycloalkoxy, C3-C7 cycloalkylmethoxy, fluorinated C1-C4 alkoxy; or R2/R3 = C1-C2 alkylenedioxy group; R4 = H, halo, NO2, C1-C4 alkyl, CF3, C1-C4 alkoxy; R5 = H or C1-C8 alkyl; R6 = H, C1-C8 alkylcarbonyl, C3-C7 cycloalkylcarbonyl, C3-C7 cycloalkylmethylcarbonyl, C1-C4 arylcarbonyl, arylalkylcarbonyl; n = 1-2] were prepared as PDE3/4 inhibitors for the treatment of respiratory disorders and/or dermatoses. Thus, reaction of 4-{(4aR,10bS)-9-ethoxy-8-methoxy-2-methyl-1,2,3,4,4a,10b-hexahydrobenzo[c][1,6]naphthyridin-6-yl}benzoic acid with phenyl-acetic acid (S)-2-isopropylamino-Pr ester hydrochloride yielded compound II. The latter inhibits PDE4 and PDE3 with -log IC50 = 9.8, 7.3 mol/L, resp.

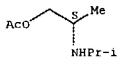
ACCESSION NUMBER: 2004:220332 CAPLUS
DOCUMENT NUMBER: 140:270839
TITLE: Preparation of phenylbenzonaphthyridine derivatives as PDE3/4 inhibitors
INVENTOR(S): Flockerzi, Dieter; Hummel, Rolf-peter; Reutter, Felix; Flockerzi, Dieter; Hummel, Rolf-peter; Reutter, Felix
PATENT ASSIGNEE(S): Altana Pharma Ag, Germany
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

L10 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004022557	A1	20040318	WO 2003-EP9617	20030829
W: AE, AL, AU, BA, BR, CA, CN, CO, DZ, EC, GE, HR, ID, IL, IN, IS, JP, KR, LT, LV, MA, MK, MX, NO, NZ, PH, PL, SG, TN, UA, US, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
PRIORITY APPLN. INFO.:			EP 2002-19904	A 20020904
			US 2002-407689P	P 20020904

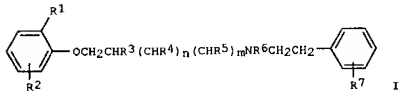
OTHER SOURCE(S): MARPAT 140:270839
IT **671821-81-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenylbenzonaphthyridine derivs. as PDE3/4 inhibitors)
RN 671821-81-1 CAPLUS
CN 1-Propanol, 2-[(1-methylethyl)amino]-, acetate (ester), (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I

AB Title compds. [I; R1, R2 = H, halo, alkyl; R3, R4, R5 = H, alkyl; R6 = H, alkyl, benzyl; R7 = NO2, amino optionally monosubstituted by alkyl, benzoyl, alkylcarbonyl, alkylsulfonyl, alkylcarbamoyl, alkylthiocarbamoyl; m, n = 0, 1; with a proviso], were prepared Thus, N-methyl-2-(2,6-dimethylphenoxy)-1-methylethylamine and 4-nitrophenethyl bromide were refluxed in Me2CHOH to give N-[2-(2,6-dimethylphenoxy)-1-methylethyl]-N-methyl-2-(4-nitrophenyl)ethylamine hydrochloride. This was hydrogenated over Pd/C in Me2CHOH to give N-[2-(2,6-dimethylphenoxy)-1-methylethyl]-N-methyl-2-(4-aminophenyl)ethylamine, which was treated with MeSO2Cl/Et3N in CH2Cl2 to give N-[4-[2-(N-methyl-N-[2-(2,6-dimethylphenoxy)-1-methylethyl]amino]ethyl]phenyl]methanesulfonamide hydrochloride. The latter at 25 mg/kg orally in rats gave an arrhythmia score of 3.94, vs. 5.6 for controls.

ACCESSION NUMBER: 1999:388155 CAPLUS
DOCUMENT NUMBER: 131:44657
TITLE: Preparation of phenoxyalkylaminoethylarenes as antiarrhythmic compounds.
INVENTOR(S): Papp, Gyula; Varro, Andras; Matyus, Peter; Varga, Ildiko; Rettegi, Tivadar; Druga, Alice; Simay, Antal; Moravcsik, Imre; Berzsenyi, Pal; Barlocco, Daniella; Cignarella, Giorgio; Patfalusi, Marta
PATENT ASSIGNEE(S): Gyogyszerkutato Intezet Kft., Hung.; Szent-Gyorgyi Albert Orvostudomanyi Egyetem
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

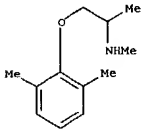
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9929655	A1	19990617	WO 1998-HU101	19981210
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2313191	AA	19990617	CA 1998-2313191	19981210
AU 9916789	A1	19990628	AU 1999-16789	19981210
AU 738672	B2	20010920		

L10 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

EP 1037871	A1	20000927	EP 1998-961331	19981210
EP 1037871	B1	20020703		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
BR 9814270	A	20011016	BR 1998-14270	19981210
JP 2001525388	T2	20011211	JP 2000-524252	19981210
AT 220058	E	20020715	AT 1998-961331	19981210
NZ 504982	A	20020726	NZ 1998-504982	19981210
RU 2193024	C2	20021120	RU 2000-118325	19981210
PT 1037871	T	20021129	PT 1998-961331	19981210
ES 2179547	T3	20030116	ES 1998-961331	19981210
NO 2000002946	A	20000807	NO 2000-2946	20000608
US 6265445	B1	20010724	US 2000-555602	20000728
PRIORITY APPLN. INFO.:			HU 1997-2411	A 19971211
			WO 1998-HU101	W 19981210

OTHER SOURCE(S): MARPAT 131:44657
IT **128942-29-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenoxyalkylaminoethylarenes as antiarrhythmics)
RN 128942-29-0 CAPLUS
CN 2-Propanamine, 1-(2,6-dimethylphenoxy)-N-methyl-, (-)- (9CI) (CA INDEX NAME)

Rotation (-).



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

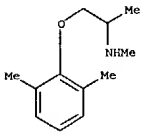
AB Perpentylated and partially pentylated and acetylated α- and β-cyclodextrins were used as chiral stationary phases for capillary gas chromatog. Enantiomeric separation of natural compds., flavor constituents, pheromones, pharmaceuticals and enantioselective chemical reaction products for stereochem. anal. is proposed.

ACCESSION NUMBER: 1990:583987 CAPLUS
DOCUMENT NUMBER: 113:183987
TITLE: Enantioselective capillary gas chromatography with modified cyclodextrins as chiral stationary phases
AUTHOR(S): Koenig, Wilfried A.; Lutz, Sabine; Wenz, Gerhard
CORPORATE SOURCE: Inst. Org. Chem., Univ. Hamburg, Hamburg, D-2000/13, Fed. Rep. Ger.
SOURCE: Proc. Int. Symp. Cyclodextrins, 4th (1988), 465-71. Editor(s): Huber, O.; Szejtli, Jozsef. Kluwer: Dordrecht, Neth.
CODEN: 56SBAU
DOCUMENT TYPE: Conference
LANGUAGE: English

IT **128942-29-0**
RL: ANST (Analytical study); PROC (Process)
(separation of, from enantiomer by capillary gas chromatog. after trifluoroacetylation, on modified cyclodextrin chiral stationary phase)

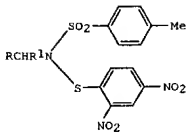
RN 128942-29-0 CAPLUS
CN 2-Propanamine, 1-(2,6-dimethylphenoxy)-N-methyl-, (-)- (9CI) (CA INDEX NAME)

Rotation (-).



L10 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

GI



I

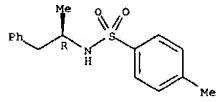
AB The absolute configuration of chiral primary amines RCHR1NH2 [R = Me, Et; R1 = Et, Me(CH2)4, Me3C, Ph, p-BrC6H4, PhCH2, α-naphthyl] were determined from the optical rotation (ORD) of the corresponding sulfenylsulfonamide derivs. I. The chiral center in the amine moiety induces asymmetry at the sulfenamide chiral axis by shifting the equilibrium between diastereomers.

ACCESSION NUMBER: 1984:629552 CAPLUS
DOCUMENT NUMBER: 101:229552
TITLE: Stereochemistry of trivalent nitrogen compounds. 39. Thermodynamic asymmetric induction: a new approach to the development of rules for the determination of absolute configurations
AUTHOR(S): Raban, Morton; Moulin, Christophe P.; Lauderback, Sanford K.; Swilley, Brian
CORPORATE SOURCE: Dep. Chem., Wayne State Univ., Detroit, MI, 48202, USA
SOURCE: Tetrahedron Letters (1984), 25(32), 3419-22
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **72938-94-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, optical rotation, and derivatization of)

RN 72938-94-4 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-(1-methyl-2-phenylethyl)-, (R)- (9CI) (CA INDEX NAME)

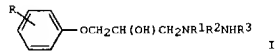
Absolute stereochemistry.



L10 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L10 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

GI



I

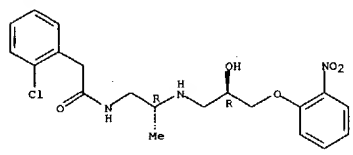
AB The title compds. I (R = H, Cl, CN, Me, NO2, CH:CHOCH2, Ac, vinyl, AcO; R1 = H or Me; R2 = CH2, C1-3 alkylene, or propylene; R3 = HCO, Ac, acyl, carbamoyl, substituted carbamoyl, and alkyl- or arylsulfonyl) were mostly prepared by cleavage of the appropriate epoxyphenoxypropane with the corresponding amide. Many compds. were more potent than propranolol as β-blockers, yet showed a cardioselectivity comparable to that of practolol in the anesthetized cat. Structure activity relations are discussed.

ACCESSION NUMBER: 1982:555937 CAPLUS
DOCUMENT NUMBER: 97:155937
TITLE: β-Adrenergic blocking agents. 22. 1-Phenoxy-3-[[(substituted-amido)alkyl]amino]-2-propanols
AUTHOR(S): Large, M. S.; Smith, L. H.
CORPORATE SOURCE: Pharm. Div., Imp. Chem. Ind. PLC, Alderley Park/Macclesfield/Cheshire, UK
SOURCE: Journal of Medicinal Chemistry (1982), 25(11), 1286-92
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:155937

IT **83029-56-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cardioselective sympatholytic activity of)

RN 83029-56-5 CAPLUS
CN Benzeneacetamide, 2-chloro-N-[2-[[2-hydroxy-3-(2-nitrophenoxy)propyl]amino]propyl]-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L10 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

AB ORD (and in some cases CD) spectra are presented for 11 RSN(SO2C6H4Me-4)CHMeR1 (R = CCl3, 4-chloro-2-methylphenyl, 2-nitrophenyl, 2,4-dinitrophenyl; R1 = Ph, 1-naphthyl, benzyl). A number of the spectra exhibit intense Cotton effects characteristic of inherently dissym. chromophores near 200 nm. The configuration at the asym. C seems to be related to the sign of long-wavelength transition (near 350 mn) in the 2,4-dinitrobenzenesulfenamides. This is ascribed to an equilibrium asym. induction from the asym. center into the sulfenamide chiral axis, whose configuration is reflected by the sign of this Cotton effect. Examination of such derivs. may provide a useful method for determination of the absolute configuration of amines.

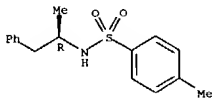
ACCESSION NUMBER: 1980:445786 CAPLUS
DOCUMENT NUMBER: 93:45786
TITLE: Chiroptical properties of sulfenamides
AUTHOR(S): Raban, M.; Lauderback, S. K.
CORPORATE SOURCE: Dep. Chem., Wayne State Univ., Detroit, MI, 48202, USA
SOURCE: Journal of Organic Chemistry (1980), 45(13), 2636-41
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **72938-94-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with sulfenyl chlorides)

RN 72938-94-4 CAPLUS

CN Benzenesulfonamide, 4-methyl-N-(1-methyl-2-phenylethyl)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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FULL ESTIMATED COST                                       30.29      37.01

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)              SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                       -4.16      -4.16

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STRUCTURE FILE UPDATES:     4 MAY 2004  HIGHEST RN 679784-15-7
DICTIONARY FILE UPDATES:    4 MAY 2004  HIGHEST RN 679784-15-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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Uploading C:\Program Files\Stnexp\Queries\09857465.str
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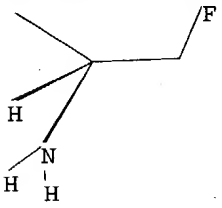

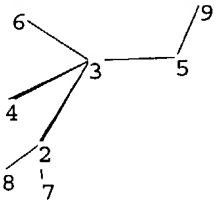


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chain bonds :
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exact/norm bonds :
2-3
exact bonds :
2-7  2-8  3-4  3-5  3-6  5-9


G1:H,F

Match level :
2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:CLASS  9:CLASS

Stereo Bonds:
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3-2 (Single Wedge).
4-3 (Single Hash).

Stereo Chiral Centers:

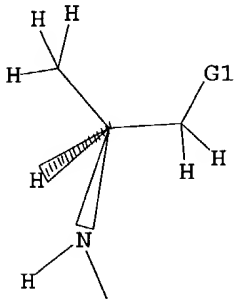
3 (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 3

L11 STRUCTURE UPLOADED

=> d query
L11 STR



G1 H,F

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 115497 TO ITERATE

0.9% PROCESSED 1000 ITERATIONS 4 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 7950

L12 4 SEA SSS SAM L11

=> s l11 full
FULL SEARCH INITIATED 16:50:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 17.3% PROCESSED 400000 ITERATIONS 1512 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.13

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                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS    8457

L13         1512 SEA SSS FUL L11

=> fil caplus
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
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FULL ESTIMATED COST                                     155.42     192.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)            SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                       0.00      -4.16

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FILE COVERS 1907 - 5 May 2004  VOL 140 ISS 19
FILE LAST UPDATED: 4 May 2004  (20040504/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l13
L14         262 L13

=> d l14 200-262 abs ibib hitstr
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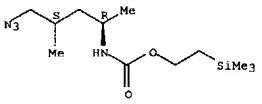
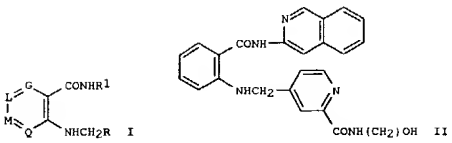
L14 ANSWER 200 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB A set of three-armed urea-containing anion receptors was prepared The receptors
all have the same binding topol. but differ in the level of conformational
preorganization with respect to the arrangement of the side-arms relative to the platform and within the side arms themselves. This is mirrored in a specific increase (+2.5) in the binding constant for chloride and in a 12-fold increase in the chloride/nitrate-selectivity.
ACCESSION NUMBER: 2002:876129 CAPLUS
DOCUMENT NUMBER: 138:187254
TITLE: Effect of conformational preorganization of a three-armed host on anion binding and selectivity
AUTHOR(S): Hettche, Frank; Reiss, Philipp; Hoffmann, Reinhard W.
CORPORATE SOURCE: Fachbereich Chemie der Philipps Universitat Marburg, Marburg, 35032, Germany
SOURCE: Chemistry--A European Journal (2002), 8(21), 4946-4956
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:187254
IT **499101-26-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(phthaloylation; effect of conformational preorganization of a three-armed host on anion binding and selectivity)
RN 499101-26-7 CAPLUS
CN Carbamic acid, [(1R,3S)-4-azido-1,3-dimethylbutyl]-, 2-(trimethylsilyl)ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 201 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI



AB Title compds. I [G, L, M, Q = N, (un)substituted CH, ≤1 of them being N; R = (un)substituted N heterocycle; R1 = (un)substituted alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, heteroaryl] were prepared I are inhibitors of VEGFR-2 and VEGFR-3 and are used as medicaments for treating
diseases that are caused by persistent angiogenesis, such as psoriasis, Kaposi's sarcoma, restenosis, such as e.g. stent-induced restenosis, endometriosis, Crohn's disease, Hodgkin's disease, leukemia, arthritis, such as rheumatoid arthritis, hemangioma, angiofibromatosis, in eye diseases such as diabetic retinopathy, neovascular glaucoma, in kidney diseases such as glomerulonephritis, diabetic nephropathy, malign nephrosclerosis, thrombic micro-angiopathic syndrome, transplant rejection
and glomerulopathy, in fibrotic diseases such as hepatic cirrhosis, mesangial-cell proliferative diseases, arteriosclerosis, damage to the nerve tissue and inhibition of the re-occlusion of vessels after balloon catheter treatment, in vessel prosthetics or after the use of mech. devices for keeping vessels open, e.g. stents, as immunosuppressants, to support wound healing without scars and in cases of age spots and contact dermatitis. I can also be used as inhibitors of VEGFR-3 in lymphangiogenesis for hyperplastic and dysplastic changes in the lymphatic
system. Thus, 2-amino-N-isoquinolin-3-ylbenzamide was treated with 2-bromo-5-pyridinecarboxaldehyde, followed by carboxylaton and amidation to give the amide II. II had IC50 for inhibition of VEGFR-2 of 40 nM and for inhibition of cytochrome 450 isoenzyme 2C9 of 2.9 μM.
ACCESSION NUMBER: 2002:868928 CAPLUS
DOCUMENT NUMBER: 137:352900
TITLE: Selective anthranilamide pyridine amides as inhibitors
of VEGFR-2 and VEGFR-3
INVENTOR(S): Ernst, Alexander; Huth, Andreas; Krueger, Martin; Thierauch, Karl-Heinz; Menrad, Andreas; Haberey, Martin
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 115 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002090352	A2	20021114	WO 2002-EP4924	20020503
WO 2002090352	A3	20030501		
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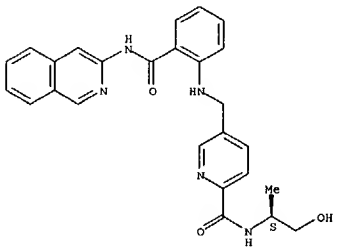
DE 10125294	A1	20021121	DE 2001-10125294	20010515
DE 10164590	A1	20030710	DE 2001-10164590	20011221
EP 1392680	A2	20040303	EP 2002-735333	20020503
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.: DE 2001-10123574 A 20010508
DE 2001-10125294 A 20010515
DE 2001-10164590 A 20011221
WO 2002-EP4924 W 20020503

OTHER SOURCE(S): MARPAT 137:352900
IT **474798-02-2P 474798-03-3P 474798-18-0P**
474798-19-1P 474798-48-6P 474798-49-7P
474798-58-8P 474798-59-9P 474798-70-4P
474798-71-5P 474798-77-1P 474798-78-2P
474799-02-5P 474799-03-6P 474799-06-9P
474799-07-0P 474799-08-1P 474799-10-5P
474799-12-7P 474799-13-8P 474799-17-2P
474799-18-3P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoquinolinylcarbamoylphenylaminomethylpyridinecarboxamides as VEGFR-2 and VEGFR-3 inhibitors)
RN 474798-02-2 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1S)-2-hydroxy-1-methylethyl]-5-[[[2-[(3-isoquinolinylamino)carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

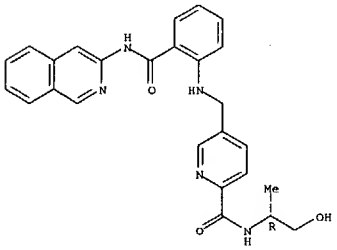
Absolute stereochemistry.

L14 ANSWER 201 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



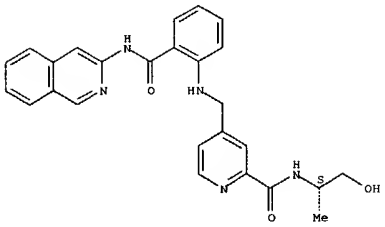
RN 474798-03-3 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1R)-2-hydroxy-1-methylethyl]-5-[[[2-[(3-isoquinolinylamino)carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



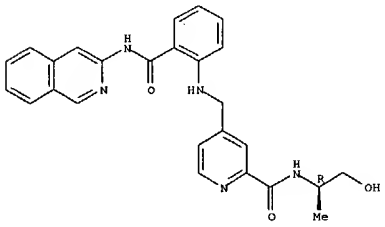
RN 474798-18-0 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1S)-2-hydroxy-1-methylethyl]-4-[[[2-[(3-isoquinolinylamino)carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



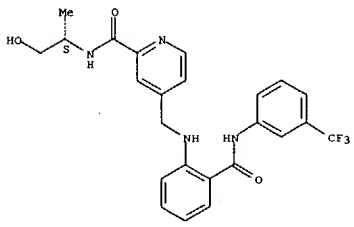
RN 474798-19-1 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1R)-2-hydroxy-1-methylethyl]-4-[[[2-[(3-isoquinolinylamino)carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



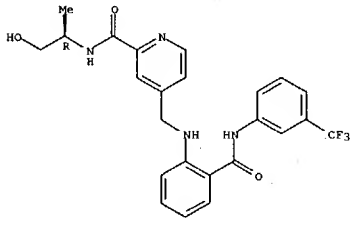
RN 474798-48-6 CAPLUS
CN 2-Pyridinecarboxamide,
4-[[[2-[(3-isoquinolinylamino)carbonyl]phenyl]amino]methyl]-N-[(1R)-2-methoxy-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 474798-59-9 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1R)-2-hydroxy-1-methylethyl]-4-[[[2-[[[3-(trifluoromethyl)phenyl]amino]carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 474798-70-4 CAPLUS
CN 2-Pyridinecarboxamide,
4-[[[3-fluoro-2-[(3-isoquinolinylamino)carbonyl]phenyl]amino]methyl]-N-[(1S)-2-hydroxy-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474798-49-7 CAPLUS
CN 2-Pyridinecarboxamide,
4-[[[2-[(3-isoquinolinylamino)carbonyl]phenyl]amino]methyl]-N-[(1S)-2-methoxy-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474798-58-8 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1S)-2-hydroxy-1-methylethyl]-4-[[[2-[[[3-(trifluoromethyl)phenyl]amino]carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

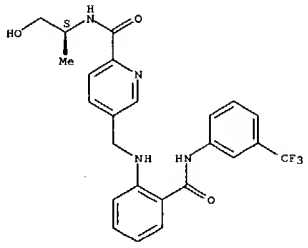
Absolute stereochemistry.

RN 474798-71-5 CAPLUS
CN 2-Pyridinecarboxamide,
4-[[[3-fluoro-2-[(3-isoquinolinylamino)carbonyl]phenyl]amino]methyl]-N-[(1R)-2-hydroxy-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

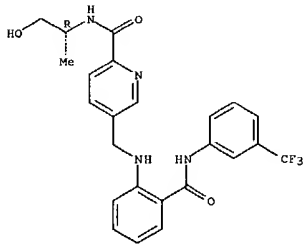
RN 474798-77-1 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1S)-2-hydroxy-1-methylethyl]-5-[[[2-[[[3-(trifluoromethyl)phenyl]amino]carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



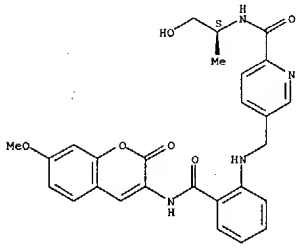
RN 474798-78-2 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1R)-2-hydroxy-1-methylethyl]-5-[[[2-[[[3-(trifluoromethyl)phenyl]amino]carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



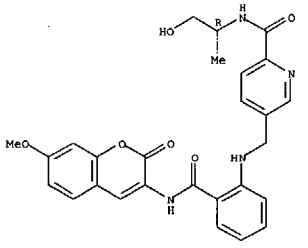
RN 474799-02-5 CAPLUS
CN 2-Pyridinecarboxamide, 5-[[[2-[[(2,3-dihydro-2-oxo-1H-indol-5-yl)amino]carbonyl]phenyl]amino]methyl]-N-[(1S)-2-hydroxy-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



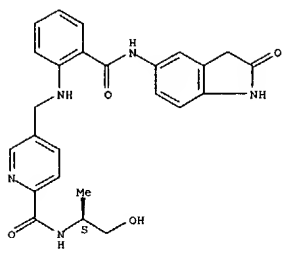
RN 474799-07-0 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1R)-2-hydroxy-1-methylethyl]-5-[[[2-[[(7-methoxy-2-oxo-2H-1-benzopyran-3-yl)amino]carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



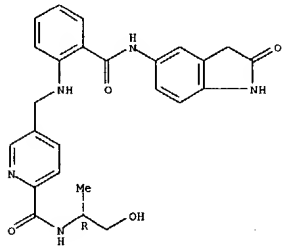
RN 474799-08-1 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1R)-2-hydroxy-1-methylethyl]-5-[[[2-[[(7-methoxy-3-methyl-2-quinolinyl)amino]carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



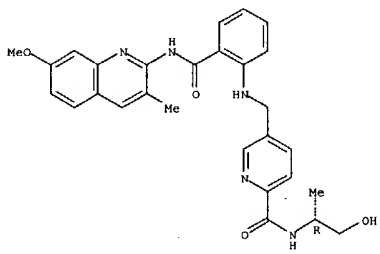
RN 474799-03-6 CAPLUS
CN 2-Pyridinecarboxamide, 5-[[[2-[[(2,3-dihydro-2-oxo-1H-indol-5-yl)amino]carbonyl]phenyl]amino]methyl]-N-[(1R)-2-hydroxy-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



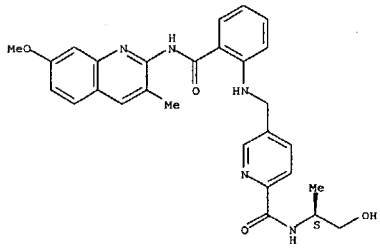
RN 474799-06-9 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1S)-2-hydroxy-1-methylethyl]-5-[[[2-[[(7-methoxy-2-oxo-2H-1-benzopyran-3-yl)amino]carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



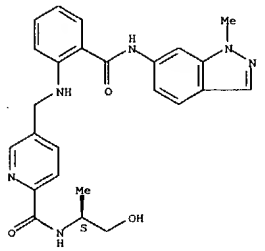
RN 474799-10-5 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1S)-2-hydroxy-1-methylethyl]-5-[[[2-[[(7-methoxy-3-methyl-2-quinolinyl)amino]carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



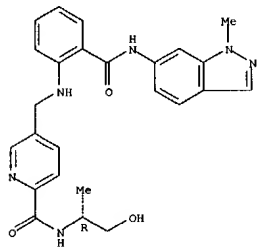
RN 474799-12-7 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1S)-2-hydroxy-1-methylethyl]-5-[[[2-[[(1-methyl-1H-indazol-6-yl)amino]carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



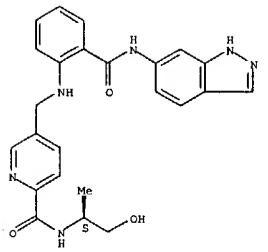
RN 474799-13-8 CAPLUS
CN 2-Pyridinecarboxamide,
N-[(1R)-2-hydroxy-1-methylethyl]-5-[[[2-[[(1-methyl-1H-indazol-6-yl)amino]carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



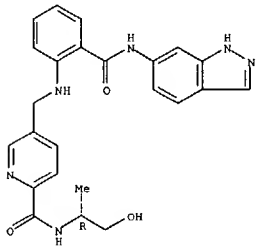
RN 474799-17-2 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1S)-2-hydroxy-1-methylethyl]-5-[[[2-[(1H-indazol-6-ylamino)carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

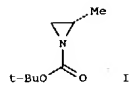


RN 474799-18-3 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1R)-2-hydroxy-1-methylethyl]-5-[[[2-[(1H-indazol-6-ylamino)carbonyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI



I

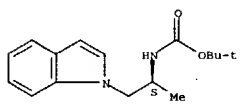
AB An improved process for the N-alkylation of indoles using N-protected homochiral aziridine I has been developed. This procedure allows reduced quantities of homochiral starting material to be used and leads to improved overall yields and operability.

ACCESSION NUMBER: 2002:863131 CAPLUS
DOCUMENT NUMBER: 138:106567
TITLE: An Improved Process for the N-Alkylation of Indoles Using Chiral N-Protected 2-Methylaziridines
AUTHOR(S): Giles, Paul R.; Rogers-Evans, Mark; Soukup, Milan; Knight, John
CORPORATE SOURCE: Vernalis Research Ltd., Winnersh, Wokingham, RG41 5UA, UK
SOURCE: Organic Process Research & Development (2003), 7(1), 22-24
CODEN: OPRDFK; ISSN: 1083-6160
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:106567

IT **486404-38-0P 502689-73-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(N-alkylation of indoles using chiral N-protected methylaziridines)

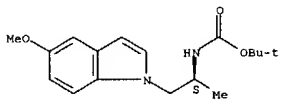
RN 486404-38-0 CAPLUS
CN Carbamic acid, [(1S)-2-(1H-indol-1-yl)-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



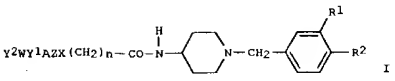
RN 502689-73-8 CAPLUS
CN Carbamic acid, [(1S)-2-(5-methoxy-1H-indol-1-yl)-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 203 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I

AB The title compds. I [R1, R2 = H, halo; etc.; n = 1 - 5; X = bond, O, etc.;
Z = bond, aryl, etc.; Y1 = bond, CO, etc.; A = aryl, etc.; W = aryl, etc.;
Y2 = amino, etc.] are prepared The bioactivities of compds. of this invention were demonstrated.

ACCESSION NUMBER: 2002:849618 CAPLUS
DOCUMENT NUMBER: 137:370092
TITLE: Preparation of benzylpiperidine derivatives as chemokine inhibitors
INVENTOR(S): Kiuchi, Masatoshi; Kuroita, Takanobu; Tomozane, Hideo;
Takeda, Shuuzou; Tanaka, Yoshihito; Higashi, Hidemitsu; Kuwahara, Shigeki
PATENT ASSIGNEE(S): Mitsubishi Pharma Corporation, Japan
SOURCE: PCT Int. Appl., 231 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002088111	A1	20021107	WO 2002-JP4291	20020426

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1389616	A1	20040218	EP 2002-722878	20020426

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

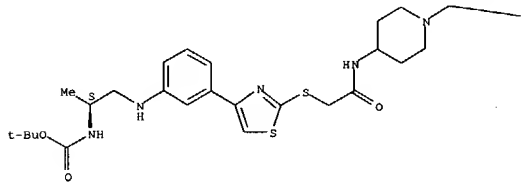
PRIORITY APPLN. INFO.: JP 2001-132853 A 20010427
JP 2001-277139 A 20010912
WO 2002-JP4291 W 20020426

OTHER SOURCE(S): MARPAT 137:370092
IT **474969-57-8P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of benzylpiperidine derivs. as chemokine inhibitors)
RN 474969-57-8 CAPLUS

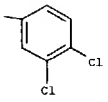
L14 ANSWER 203 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN Carbamic acid, [(1S)-2-[[3-[2-[[2-[[1-[(3,4-dichlorophenyl)methyl]-4-piperidinyl]amino]-2-oxoethyl]thio]-4-thiazolyl]phenyl]amino]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

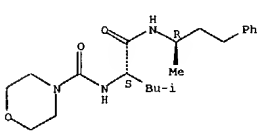


REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 204 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB The specificity of the immune response relies on processing of foreign proteins and presentation of antigenic peptides at the cell surface. Inhibition of antigen presentation, and the subsequent activation of T-cells, should, in theory, modulate the immune response. The cysteine protease cathepsin S performs a fundamental step in antigen presentation and therefore represents an attractive target for inhibition. Herein, the
authors report a series of potent and reversible Cathepsin S inhibitors based on dipeptide nitriles. These inhibitors show nanomolar inhibition of the target enzyme as well as cellular potency in a human B cell line. The first x-ray crystal structure of a reversible inhibitor cocrystd. with
cathepsin S is also reported.

ACCESSION NUMBER: 2002:835002 CAPLUS
DOCUMENT NUMBER: 138:56234
TITLE: Design and synthesis of dipeptide nitriles as reversible and potent cathepsin S inhibitors
AUTHOR(S): Ward, Yancey D.; Thomson, David S.; Frye, Leah L.; Cywin, Charles L.; Morwick, Tina; Emmanuel, Michel J.;
Zindell, Renee; McNeil, Daniel; Bekkali, Younes; Giradot, Marc; Hrapchak, Matt; DeTuri, Molly; Crane, Kathy; White, Della; Pav, Susan; Wang, Yong; Hao, Ming-Hong; Grygon, Christine A.; Labadia, Mark E.; Freeman, Dorothy M.; Davidson, Walter; Hopkins, Jerry L.; Brown, Maryanne L.; Spero, Denice M.
CORPORATE SOURCE: Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877-0368, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(25), 5471-5482
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:56234
IT **479091-47-9P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and biol. activity of dipeptide nitriles as reversible and
potent cathepsin S inhibitors)
RN 479091-47-9 CAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-3-methyl-1-[[[(1R)-1-methyl-3-phenylpropyl]amino]carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 204 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L14 ANSWER 205 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

AB Among the active-site residues of scytalone dehydratase, the side-chain carboxamide of asparagine 131 has the greatest potential for strong electrostatic interactions. Structure-based inhibitor design aimed at enhancing interactions with this residue led to the synthesis of a series of highly potent inhibitors that have a five- or six-membered ring containing a carbonyl functionality for hydrogen bonding. To achieve a good orientation for hydrogen bonding, the inhibitors incorporate a Ph substituent that displaces a phenylalanine residue away from the five- or six-membered rings. Without the Ph substituent, inhibitor binding potency is diminished by three orders of magnitude. Larger Ki values of a site-directed mutant (Asn131Ala) of scytalone dehydratase in comparison to those of wild-type enzyme validate the design concept. The most potent inhibitor (Ki= 15 pM) contains a tetrahydrothiophenone that can form a single hydrogen bond with the asparagine carboxamide. Inhibitors with a butyrolactam that can form two hydrogen bonds with the asparagine carboxamide demonstrate excellent in vivo fungicidal activity.

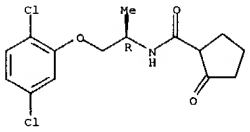
ACCESSION NUMBER: 2002:823392 CAPLUS
DOCUMENT NUMBER: 138:299663
TITLE: Design of inhibitors of scytalone dehydratase: probing interactions with an asparagine carboxamide
AUTHOR(S): Basarab, Gregory S.; Jordan, Douglas B.; Gehret, Troy C.; Schwartz, Rand S.
CORPORATE SOURCE: Experimental Station, DuPont Central Research & Development, Wilmington, DE, 19880, USA
SOURCE: Bioorganic & Medicinal Chemistry (2002), 10(12), 4143-4154
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:299663

IT **508213-72-7P**
RL: AGR (Agricultural use); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(product/enzyme inhibitor/fungicidal; preparation of cyclic carboxamides as inhibitors of scytalone dehydratase wild-type and mutant forms in relation to fungicides for control of rice blast disease)

RN 508213-72-7 CAPLUS
CN Cyclopentanecarboxamide, N-[(1R)-2-(2,5-dichlorophenoxy)-1-methylethyl]-2-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 205 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 206 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

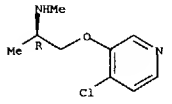
AB Analogs of the potent nicotinic receptor agonist 3-(2-aminoethoxy)pyridine substituted at the 5' and 6'-positions of the pyridine ring were synthesized and tested in vitro for nicotinic receptor binding activity (displacement of [3H](-)cytisine from whole rat brain synaptic membranes). The substituted analogs exhibited Ki values ranging from 0.076 to 319 nM compared to a Ki value of 26 nM for previously identified A-84543. Among the compds. tested, 5'-vinyl-6'-chloro substituted A-84543 was the most potent.

ACCESSION NUMBER: 2002:808837 CAPLUS
DOCUMENT NUMBER: 138:187613
TITLE: Synthesis and biological evaluation of pyridine-modified analogues of 3-(2-Aminoethoxy)pyridine as novel nicotinic receptor ligands
AUTHOR(S): Lin, Nan-Horng; Dong, Liming; Bunnelle, William H.; Anderson, David J.; Meyer, Michael D.
CORPORATE SOURCE: Pharmaceutical Products Division, Neurological and Urological Diseases Research, Abbott Laboratories, Abbott Park, IL, 60064-3500, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(22), 3321-3324
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:187613

IT **497949-17-4P 497949-18-5P 497949-19-6P 497949-20-9P 497949-21-0P 497949-22-1P 497949-23-2P 497949-24-3P 497949-25-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn of pyridine analogs of 3-(2-aminoethoxy)pyridine from α-amino carboxylic acids and evaluation of their activity as nicotinic receptor ligands)

RN 497949-17-4 CAPLUS
CN 2-Propanamine, 1-[(4-chloro-3-pyridinyl)oxy]-N-methyl-, (2R)- (9CI) (CA INDEX NAME)

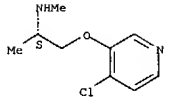
Absolute stereochemistry.



RN 497949-18-5 CAPLUS
CN 2-Propanamine, 1-[(4-chloro-3-pyridinyl)oxy]-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

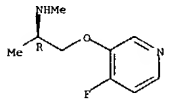
Absolute stereochemistry.

L14 ANSWER 206 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



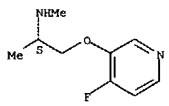
RN 497949-19-6 CAPLUS
CN 2-Propanamine, 1-[(4-fluoro-3-pyridinyl)oxy]-N-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



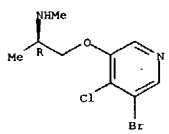
RN 497949-20-9 CAPLUS
CN 2-Propanamine, 1-[(4-fluoro-3-pyridinyl)oxy]-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 497949-21-0 CAPLUS
CN 2-Propanamine, 1-[(5-bromo-4-chloro-3-pyridinyl)oxy]-N-methyl-, (2R)- (9CI) (CA INDEX NAME)

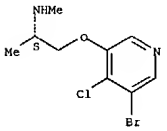
Absolute stereochemistry.



RN 497949-22-1 CAPLUS
CN 2-Propanamine, 1-[(5-bromo-4-chloro-3-pyridinyl)oxy]-N-methyl-, (2S)-

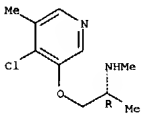
L14 ANSWER 206 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



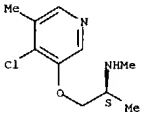
RN 497949-23-2 CAPLUS
CN 2-Propanamine, 1-[(4-chloro-5-methyl-3-pyridinyl)oxy]-N-methyl-, (2R)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 497949-24-3 CAPLUS
CN 2-Propanamine, 1-[(4-chloro-5-methyl-3-pyridinyl)oxy]-N-methyl-, (2S)-
(9CI) (CA INDEX NAME)

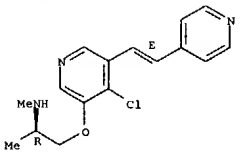
Absolute stereochemistry.



RN 497949-25-4 CAPLUS
CN 2-Propanamine, 1-[[4-chloro-5-[(1E)-2-(4-pyridinyl)ethenyl]-3-
pyridinyl]oxy]-N-methyl-, (2R)- (9CI) (CA INDEX NAME)

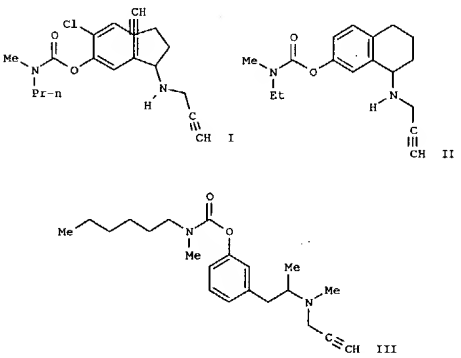
Absolute stereochemistry.
Double bond geometry as shown.

L14 ANSWER 206 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 207 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI

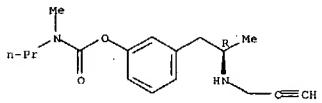


AB Carbamate derivs. of N-propargylaminoindanes (Series I) and
N-propargylphenethylamines (Series II) were synthesized via multistep
procedures from the corresponding hydroxy precursors. The resp.
rasagiline- and selegiline-related series were designed to combine
inhibitory activities of both acetylcholine esterase (AChE) and monoamine
oxidase (MAO) by virtue of their carbamoyl and propargylamine
pharmacophores. Each compound was tested for these activities in vitro
in
order to find mols. with similar potencies against each enzyme. Compds.
with such dual AChE and MAO inhibitory activities are expected to have
potential for the treatment of Alzheimer's disease. The observed SAR
also
offers insight into the requirements of the active sites on these
enzymes.
A carbamate moiety was found to be essential for AChE inhibition, which
was absent in the corresponding hydroxy precursors. The propargyl group
caused 2-70-fold decrease in AChE inhibitory activity (depending on the
position of the carbamoyl group) of Series I, but had little or no effect
in Series II. Thus, the 6- and 7-carbamyloxyphenyls in Series I were
either equipotent to, or slightly (2- to 5-fold) less active as AChE
inhibitors than, the corresponding compds. in Series II, while the
4-carbamyloxyphenyls were more potent. The presence of the carbamate
moiety in 6- and 7-carbamyloxyphenyls of Series I, considerably decreased
MAO-A and -B inhibitory activity, compared to that of the parent hydroxy
analogs, while the opposite was true for Series II. Thus, the 6- and
7-carbamyloxyphenyls in Series I were 2-3 orders of magnitude weaker MAO

L14 ANSWER 207 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
inhibitors while the 4- carbamyloxyphenyls were equipotent with the
corresponding compds. in Series II. In both series, N-methylation of the
propargylamine enhanced the MAO (A and B equally) inhibitory activities
and decreased the AChE inhibitory activity. Two candidates belonging to
the indan and tetralin ring systems (HCl salts of I and II) and one
phenethylamine (mesylate salt of III) were identified as possible leads
for further development based on the following criteria: (a) comparable
AChE and MAO-B inhibitory activities, (b) good to moderate AChE
inhibitory
activity, and (c) lack of strong MAO-A selectivity. However, it is
likely
that these compds. will be metabolized to the corresponding phenols, with
inhibitory activities against AChE and/or MAO-A or -B, different from
those of the parent carbamates. Thus, the apparent enzyme inhibition
will
be a result of the combined inhibition of all of these individual
metabolites. The results of our ongoing in vivo screening programs will
be published elsewhere.
ACCESSION NUMBER: 2002:808526 CAPLUS
DOCUMENT NUMBER: 138:55734
TITLE: Novel Dual Inhibitors of AChE and MAO Derived from Hydroxy Aminoindan and Phenethylamine as Potential Treatment for Alzheimer's Disease
AUTHOR(S): Sterling, Jeffrey; Herzig, Yaacov; Goren, Tamar; Finkelstein, Nina; Lerner, David; Goldenberg, Willy; Miskolczi, Istvan; Molnar, Sandor; Rantal, Ferenc; Tamas, Tivadar; Toth, Gyorgy; Zagyva, Adela; Zekany, Andras; Lavian, Gila; Gross, Aviva; Friedman, Rachel; Razin, Michal; Huang, Wei; Krais, Boris; Chorev, Michael; Youdim, Moussa B.; Weinstock, Marta
CORPORATE SOURCE: Research and Development Division, Teva Pharmaceutical
Industries, Jerusalem, 91010, Israel
SOURCE: Journal of Medicinal Chemistry (2002), 45(24), 5260-5279
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:55734
IT **479206-16-1P 479206-17-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective preparation of aminoindanes with inhibitory activity toward
acetylcholine esterase and monoamine oxidase useful as anti-Alzheimer's
agents)
RN 479206-16-1 CAPLUS
CN Carbamic acid, methylpropyl-, 3-[(2R)-2-(2-propynylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

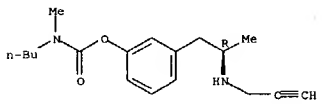
L14 ANSWER 207 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



● HCl

RN 479206-17-2 CAPLUS
CN Carbamic acid, butylmethyl-, 3-[(2R)-2-(2-propynylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

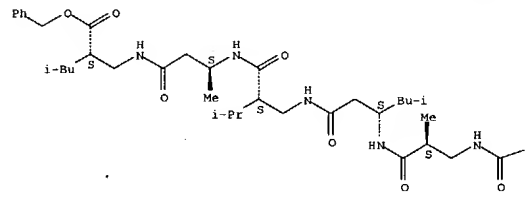
REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 208 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB The structural properties of four mixed β-peptides with alternating β2/β3- or β3/β2-sequences, R1-(S)-β3-Val-(S)-β3-Ala-(S)-β2-Leu-(R)-β3-Val-(S)-β2-Ala-(S)-β3-Leu-OR2 (R1 = tert-butoxycarbonyl, R2 = CH2Ph) (1), R1-(R)-β3-Val-(S)-β2-Ala-(S)-β3-Leu-(S)-β2-Val-(S)-β3-Ala-(S)-β2-Leu-OR2 (R1 = tert-butoxycarbonyl, R2 = CH2Ph) (2), R1-(R)-β3-Val-(S)-β2-Ala-(S)-β3-Leu-(S)-β2-Val-(S)-β3-Ala-(S)-β2-Leu-(R)-β3-Val-(S)-β2-Ala-(S)-β3-Leu-OR2 (R1 = tert-butoxycarbonyl, R2 = CH2Ph) (3), (R1 = R2 = H) (4), have been analyzed by two-dimensional homonuclear 1H-NMR- and CD spectroscopic measurements. All four β-peptides fold into (P)-helixes with twelve- and ten-membered H-bonded rings. CD Spectra of the mixed β3/β2-hexapeptide 2 and β3/β2-nonapeptide 3, indicating that peptides of this type also adopt the 12/10-helical conformation, were confirmed by NMR structural anal. For the deprotected β3/β2-nonapeptide 5d, NOEs not consistent with the 10/12 helix have been observed, showing that the stability of the helix decreases upon
N-terminal deprotection. From the NMR structures obtained, an idealized helical-wheel representation was generated, which will be used for the design of further 12/10 or 10/12 helixes.
ACCESSION NUMBER: 2002:805614 CAPLUS
DOCUMENT NUMBER: 138:153820
TITLE: Mixed β2/β3-hexapeptides and β2/β3-nonapeptides folding to (P)-helices with alternating twelve- and ten-membered hydrogen-bonded rings
AUTHOR(S): Rueping, Magnus; Schreiber, Jurg V.; Lelais, Gerald; Jaun, Bernhard; Seebach, Dieter
CORPORATE SOURCE: Laboratorium fur Organische Chemie der Eidgenossischen
Technischen Hochschule, ETH-Honggerberg, Zurich, CH-8093, Switz.
SOURCE: Helvetica Chimica Acta (2002), 85(9), 2577-2593
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:153820
IT **496862-92-1P 496862-94-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and conformation of mixed (un)protected β-peptides with alternating β2/β3- or β3/β2-sequences by two-dimensional homonuclear 1H-NMR and CD)
RN 496862-92-1 CAPLUS
CN β-Alanine, (2S)-N-[(3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-4-methyl-1-oxopentyl]-2-methyl-β-alanyl-(3S)-3-amino-5-methylhexanoyl-(2S)-2-(1-methylethyl)-β-alanyl-(3S)-3-aminobutanoyl-2-(2-methylpropyl)-, phenylmethyl ester, (2S)- (9CI) (CA INDEX NAME)

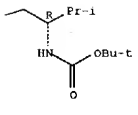
Absolute stereochemistry.

L14 ANSWER 208 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B



RN 496862-94-3 CAPLUS
CN 4,8,12,16,20,24,28,32-Octaazaheptatriacontanoic acid, 35-amino-6,19,30,36-tetramethyl-11,22-bis(1-methylethyl)-3,14,27-tris(2-methylpropyl)-5,9,13,17,21,25,29,33-octaoxo-, (3S,6S,11R,14S,19S,22S,27S,30S,35R)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

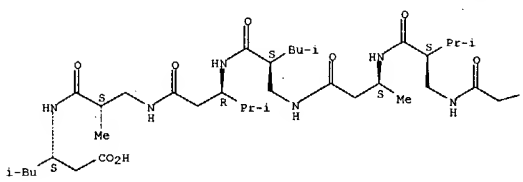
CM 1

CRN 496862-93-2
CMF C51 H95 N9 O10

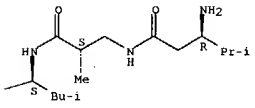
Absolute stereochemistry.

L14 ANSWER 208 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B



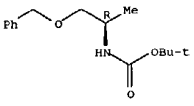
CM 2

CRN 76-05-1
CMF C2 H F3 O2

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 209 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB Addition of organometallic reagents to O-(1-phenylbutyl)benzyloxyacetaldoxime in the presence of boron trifluoride di-Et etherate is highly diastereoselective; the resulting hydroxylamines are readily converted into protected 1,2-amino alcs. and 2-hydroxymethyl nitrogen heterocycles, including the imino sugar 1,4-dideoxy-1,4-imino-D-ribitol, in high enantiomeric excess.
ACCESSION NUMBER: 2002:805157 CAPLUS
DOCUMENT NUMBER: 138:237842
TITLE: O-(1-Phenylbutyl)benzyloxyacetaldoxime, a versatile reagent for the asymmetric synthesis of protected 1,2-amino alcohols and 2-hydroxymethyl nitrogen heterocycles
AUTHOR(S): Cooper, Tracey S.; Larigo, Alexander S.; Laurent, Pierre; Moody, Christopher J.; Takle, Andrew K.
CORPORATE SOURCE: School of Chemistry, University of Exeter, Exeter, EX4 4QD, UK
SOURCE: Synlett (2002), (10), 1730-1732
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:237842
IT **502162-48-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(O-(1-phenylbutyl)benzyloxyacetaldoxime as a versatile reagent for the asym. synthesis of protected 1,2-amino alcs. and 2-hydroxymethyl nitrogen heterocycles)
RN 502162-48-3 CAPLUS
CN Carbamic acid, [(1R)-1-methyl-2-(phenylmethoxy)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

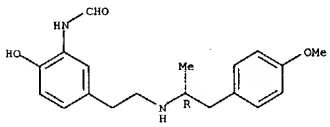
Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 210 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB The development and large-scale implementation of a novel technol. utilizing polymorphic interconversion and crystalline intermediate formation of (R,R)-formoterol L-tartrate (I) as a tool for the removal of impurities from the final product and generation of the most thermodynamically stable crystal form is reported. The crude product was generated by precipitation of the free base as the L-tartrate salt in a unique polymorphic form, form B. Warming the resultant slurry effected the formation of a partially hydrated stable crystalline intermediate, form C, with a concomitant decrease in the impurity levels in the solid. Isolation and recrystn. of form C provided I in the thermodynamically most stable polymorph, form A.
ACCESSION NUMBER: 2002:779218 CAPLUS
DOCUMENT NUMBER: 138:16525
TITLE: Taking Advantage of Polymorphism To Effect an Impurity Removal: Development of a Thermodynamic Crystal Form of (R,R)-Formoterol Tartrate
AUTHOR(S): Tanoury, Gerald J.; Hett, Robert; Kessler, Donald W.; Wald, Stephen A.; Senanayake, Chris H.
CORPORATE SOURCE: Chemical Research and Development, Sepracor Inc., Marlborough, MA, 01752, USA
SOURCE: Organic Process Research & Development (2002), 6(6), 855-862
CODEN: OPRDFK; ISSN: 1083-6160
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **477552-93-5**
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(formoterol impurity; development of thermodn. crystal form of formoterol tartrate in relation to polymorphism)
RN 477552-93-5 CAPLUS
CN Formamide, N-[2-hydroxy-5-[2-[[(1R)-2-(4-methoxyphenyl)-1-methylethyl]amino]ethyl]phenyl]- (9CI) (CA INDEX NAME)

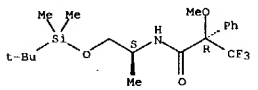
Absolute stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

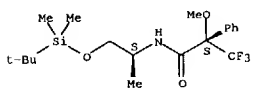
L14 ANSWER 211 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB The reversal of the relative position of 1H NMR signals observed for diastereomeric MTPA esters and amides upon addition of La(hfaa)3 (hfaa = hexafluoroacetylacetonate) can be used for verification of the validity of the correlation model employed in the modified Mosher's method. This verification extends the scope of the determination of absolute configurations using the Mosher method to substrates having only a few proton probes.
ACCESSION NUMBER: 2002:769202 CAPLUS
DOCUMENT NUMBER: 138:153173
TITLE: Use of a diamagnetic lanthanide complex for extending the scope of NMR determination of absolute configuration by the modified Mosher's method
AUTHOR(S): Omata, Kenji; Fujiwara, Tomoya; Kabuto, Kuninobu
CORPORATE SOURCE: Graduate School of Science, Department of Chemistry, Tohoku University, Aoba-ku, Sendai, 980-8578, Japan
SOURCE: Tetrahedron: Asymmetry (2002), 13(15), 1655-1662
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:153173
IT **495373-87-0P 495373-88-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(use of a diamagnetic lanthanide complex for extending the scope of NMR determination of absolute configuration by the modified Mosher's method)
RN 495373-87-0 CAPLUS
CN Benzeneacetamide, N-[(1S)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-α-methoxy-α-(trifluoromethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 495373-88-1 CAPLUS
CN Benzeneacetamide, N-[(1S)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-α-methoxy-α-(trifluoromethyl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS

L14 ANSWER 211 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

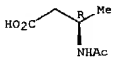
L14 ANSWER 212 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB A new diphosphine ligand bearing a hydroxy group in the backbone was synthesized starting from 9-bromocamphor. The rhodium(I) complex based on this ligand was tested in the hydrogenation of α- and β-amino acid precursors. The activity and selectivity of the catalyst were found to be strongly dependent upon the nature of the substrate. Thus, β-acetylamino carboxylates were obtained with up to 97% ee.

ACCESSION NUMBER: 2002:769196 CAPLUS
DOCUMENT NUMBER: 138:170488
TITLE: A new hydroxydiphosphine as a ligand for Rh(I)-catalyzed enantioselective hydrogenation
AUTHOR(S): Komarov, Igor V.; Monsees, Axel; Kadyrov, Renat; Fischer, Christine; Schmidt, Ute; Borner, Armin
CORPORATE SOURCE: Institut fur Organische Katalyseforschung an der Universitat Rostock e.V., Rostock, D-18055, Germany
SOURCE: Tetrahedron: Asymmetry (2002), 13(15), 1615-1620
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:170488

IT **497262-06-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and use of hydroxydiphosphine ligand for Rh(I)-catalyzed enantioselective hydrogenation in preparation of amino acids)

RN 497262-06-3 CAPLUS
CN Butanoic acid, 3-(acetylamino)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

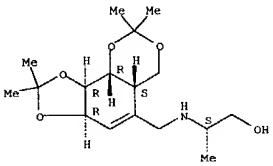
L14 ANSWER 213 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB A novel approach, which features a stereoselective 6-exo-dig radical cyclization and a palladium-catalyzed allylic amination, permits a six steps synthesis of aminocyclitol analogs from D-mannose.

ACCESSION NUMBER: 2002:769061 CAPLUS
DOCUMENT NUMBER: 138:187989
TITLE: A combined, 6-exo-dig radical cyclization-palladium catalyzed allylic amination, approach to aminocarbasugar analogs: synthesis of novel N-substituted aminocyclitols from D-mannose
AUTHOR(S): Gomez, Ana M.; Moreno, Eduardo; Valverde, Serafin; Lopez, J. Cristobal
CORPORATE SOURCE: C.S.I.C., Instituto de Quimica Organica General, Madrid, 28006, Spain
SOURCE: Tetrahedron Letters (2002), 43(44), 7863-7866
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:187989

IT **498555-18-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of aminocarbasugar analogs via stereoselective radical cyclization and palladium catalyzed allylic amination as the key steps)

RN 498555-18-3 CAPLUS
CN 1-Propanol, 2-[[[(3aR,5aS,9aR,9bR)-3a,5a,9a,9b-tetrahydro-2,2,8,8-tetramethyl-6H-1,3-dioxolo[4,5-h][1,3]benzodioxin-5-yl]methyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

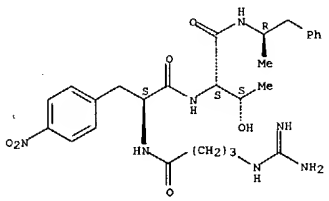
L14 ANSWER 214 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB A series of retro-binding inhibitors of human α-thrombin was prepared to elucidate structure-activity relationships (SAR) and optimize in vivo performance. Compds. 9 and 11, orally active inhibitors of thrombin catalytic activity, were identified to be efficacious in a thrombin-induced lethality model in mice.

ACCESSION NUMBER: 2002:767310 CAPLUS
DOCUMENT NUMBER: 138:378532
TITLE: Retro-Binding thrombin active site inhibitors: identification of an orally active inhibitor of thrombin catalytic activity
AUTHOR(S): Iwanowicz, Edwin J.; Kimball, S. David; Lin, James; Lau, Wan F.; Han, W.-C.; Wang, Tammy C.; Roberts, Daniel G. M.; Schumacher, W. A.; Ogletree, Martin L.; Seiler, Steven M.
CORPORATE SOURCE: Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08543-4000, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(21), 3183-3186
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **526223-46-1P**
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(retro-binding orally active inhibitors of human α-thrombin preparation and structure-activity relationship)

RN 526223-46-1 CAPLUS
CN L-Allothreoninamide, N-[4-[(aminoiminomethyl)amino]-1-oxobutyl]-4-nitro-L-phenylalanyl-N-[(1R)-1-methyl-2-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

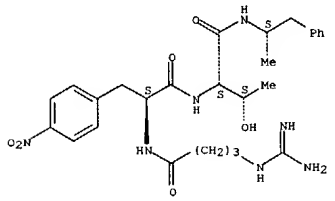


IT **526223-47-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(retro-binding orally active inhibitors of human α-thrombin preparation and structure-activity relationship)

RN 526223-47-2 CAPLUS

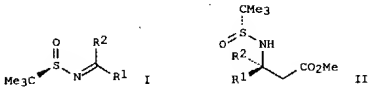
L14 ANSWER 214 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN L-Allothreoninamide, N-[4-[(aminoiminomethyl)amino]-1-oxobutyl]-4-nitro-L-phenylalanyl-N-[(1S)-1-methyl-2-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 215 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI



AB Addition of ClTi(OPr-i)3 ester enolates to tert-butanesulfinyl aldimines and
ketimines provided substituted β-amino acid derivs in high yields and with high diastereoselectivities. For example, the addition of tert-butanesulfinylimine I (R1 = Me, i-Pr, i-Bu, Ph, 3-pyridyl; R2 = H, Me) to MeCO2Me in the presence of ClTi(OPr-i)3 and LDA in THF at -78° gave β-(tert-butanesulfinylamino) acid esters II in yields > 70% and with diastereoselectivities > 95%. The N-sulfinyl-β-amino ester products were further employed as versatile reactants for both standard solution-phase and solid-phase synthetic transformations, such as the synthesis of β-peptides.

ACCESSION NUMBER: 2002:760624 CAPLUS
DOCUMENT NUMBER: 138:14170
TITLE: Asymmetric Synthesis of β-Amino Acid Derivatives Incorporating a Broad Range of Substitution Patterns by Enolate Additions to tert-Butanesulfinyl Imines
AUTHOR(S): Tang, Tony P.; Ellman, Jonathan A.
CORPORATE SOURCE: Center for New Directions in Organic Synthesis and the
Department of Chemistry, University of California, Berkeley, CA, 94720-1460, USA
SOURCE: Journal of Organic Chemistry (2002), 67(22), 7819-7832
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:14170

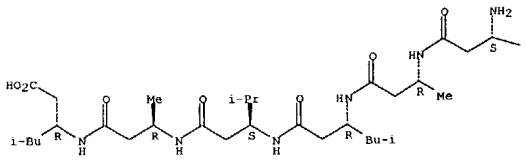
IT **477587-00-1P 477587-01-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. preparation of tert-butanesulfinyl-protected β-amino acids as intermediates for peptide synthesis)

RN 477587-00-1 CAPLUS
CN 4,8,12,16,20-Pentaazapentacosanoic acid, 23-amino-7,19,24-trimethyl-11-(1-methylethyl)-3,15-bis(2-methylpropyl)-5,9,13,17,21-pentaoxo-, (3R,7R,11S,15R,19R,23S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 215 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



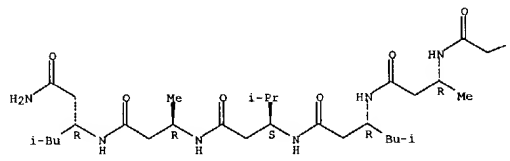
PAGE 1-B

Pr-i

RN 477587-01-2 CAPLUS
CN 4,8,12,16,20-Pentaazapentacosanamide, 23-amino-7,19,24-trimethyl-11-(1-methylethyl)-3,15-bis(2-methylpropyl)-5,9,13,17,21-pentaoxo-, (3R,7R,11S,15R,19R,23S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

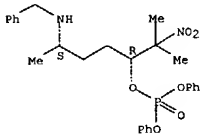
L14 ANSWER 216 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB A series of highly diastereomerically enriched 1,5-dimethyl-, 2,5-dimethyl-, and 3,5-dimethyl-N-benzyl-5-nitro-4-(diphenylphosphatoxy)hexylamines were exposed to tributyltin hydride and AIBN in benzene at reflux. The ensuing reactions, interpreted in terms of
radical denitration, radical ionic fragmentation, and nucleophilic substitution, lead to the formation of pyrrolidines with moderate to high diastereoselectivity. In five out of the six cases, the diastereoselectivity is best interpreted by backside attack by the amine on the initial contact ion pair generated by radical ionic fragmentation. In the exception that proves the rule, this mode of attack is disfavored by 1,3A strain in the initial contact ion pair, resulting in equilibration
and subsequent attack on the opposite face.

ACCESSION NUMBER: 2002:737852 CAPLUS
DOCUMENT NUMBER: 138:24610
TITLE: Diastereoselectivity in the Cyclization of Alkene Radical Cations Generated under Non-Oxidizing Conditions: Contact Ion Pairs and Memory Effects
AUTHOR(S): Crich, David; Ranganathan, Krishnakumar
CORPORATE SOURCE: Department of Chemistry, University of Illinois at Chicago, Chicago, IL, 60607-7061, USA
SOURCE: Journal of the American Chemical Society (2002), 124(42), 12422-12423
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:24610

IT **477952-53-7P 477952-54-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(contact ion pairs, memory effects, and diastereoselectivity in cyclization of alkene radical cations to pyrrolidine derivs.)

RN 477952-53-7 CAPLUS
CN Phosphoric acid, (1R,4S)-1-(1-methyl-1-nitroethyl)-4-[(phenylmethyl)amino]pentyl diphenyl ester (9CI) (CA INDEX NAME)

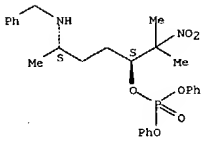
Absolute stereochemistry.



RN 477952-54-8 CAPLUS
CN Phosphoric acid, (1S,4S)-1-(1-methyl-1-nitroethyl)-4-[(phenylmethyl)amino]pentyl diphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 216 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L14 ANSWER 217 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
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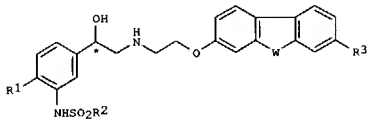


I

AB Disclosed are remedies for fatty liver containing the title compds., e.g. [I; R1 = H, halo, OH; R2 = lower alkyl, benzyl; R3 = OR, halo, CF3, lower alkyl, lower acyl, NR4R4', NO2, cyano (wherein R = H, lower alkyl, benzyl, optionally substituted lower acyl; R4, R4' = H, lower alkyl, lower acyl, benzyl, SO2R5; wherein R5 = lower alkyl, benzyl); W = O, NH, S; * denotes an asym. carbon atom] having a β3-agonistic activity. (R)-N-[5-[2-[2-(dibenzothiophen-3-yloxy)ethylamino]-1-hydroxyethyl]-2-hydroxyphenyl]methanesulfonamide hydrochloride and (R)-N-[5-[2-[2-(9H-carbazol-2-yloxy)ethylamino]-1-hydroxyethyl]-2-hydroxyphenyl]methanesulfonamide hydrochloride at 1 mg/kg per day for 4 wk lowered the triglyceride per unit of fatty liver in rat by 25 and 23%, resp.

ACCESSION NUMBER: 2002:736110 CAPLUS
DOCUMENT NUMBER: 137:262950
TITLE: Preparation of carbazole, dibenzothiophene, and dibenzofuran derivatives as remedies for fatty liver
INVENTOR(S): Umeno, Hiroshi; Kobayashi, Teruki
PATENT ASSIGNEE(S): Asahi Kasei Kabushiki Kaisha, Japan
SOURCE: PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

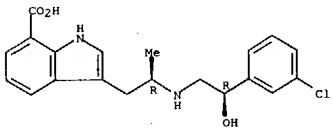
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002074306	A1	20020926	WO 2002-JP2486	20020315

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 2001-77407 A 20010319
OTHER SOURCE(S): MARPAT 137:262950

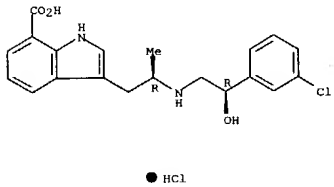
L14 ANSWER 217 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
IT **461696-25-3P 461696-29-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of carbazole, dibenzothiophene, and dibenzofuran derivs. having β3-agonistic activity as remedies for fatty liver)
RN 461696-25-3 CAPLUS
CN 1H-Indole-7-carboxylic acid, 3-[(2R)-2-[[(2R)-2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 461696-29-7 CAPLUS
CN 1H-Indole-7-carboxylic acid, 3-[(2R)-2-[[(2R)-2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

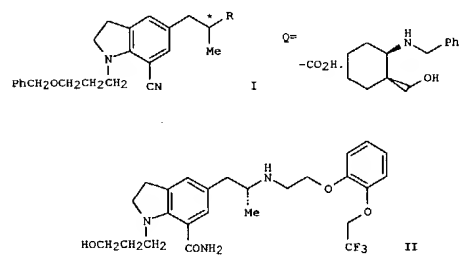
Absolute stereochemistry.



● HCl

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 218 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I II

AB The title compds. (I; R = CO2H, CONH2, NH2; Q: the carbon atom denoted by * represents the carbon atom with R or RS configuration; provided that the carbon atom denoted by * represents the carbon atom with R configuration, R is CO2H) are prepared These compds. are useful as intermediates for (R)-1-(3-hydroxypropyl)-5-[2-[2-[2-(2,2,2-trifluoroethoxy)phenoxy]ethylamino]propyl]indoline-7-carboxamide (II) which possesses selective smooth muscle relaxant activity for urinary tract and little effect on blood pressure and is useful as a therapeutic agent for dysuria. Thus, 2.00 g 3-[1-(3-benzyloxypropyl)-7-cyanoindolin-5-yl]-2-methylpropionic acid (III) and 11.6 g (1S,2R)-cis-(-)-2-benzylaminocyclohexanemethanol (IV) were dissolved in 100 mL EtOAc with heating, stirred with 1.0 g activated charcoal at room temperature for 30 min, and filtered. To the filtrate was added portionwise 100 mL hexane, followed by seeding with a diastereomer salt prepared sep., and the resulting mixture was stirred overnight at room temperature and filtered to give, after washing the crystals with hexane/EtOAc (2/1) and drying at 50 ° for 3 h, the diastereomer salt (13.4 7 g). The diastereomer salt was recrystd. from hexane/EtOAc to give 5.99 g (R)-III.IV (92.8% ee) which (5.00 g) was stirred with 50 mL 1 M aqueous HCl and 50 mL EtOAc at for 1 h and the EtOAc layer was separated, washed with aqueous NaCl, and dried over anhydrous Na2SO4, followed by distilling off th solvent to give 3.20 g (R)-III (91.8% ee). To a solution of 3.00 g (R)-III in MeCN was added 2.57 g 1,1'-carbonyldiimidazole and stirred at room temperature overnight,

L14 ANSWER 218 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
treated with a satd. NH3 soln. in MeCN (20 mL), sealed, and stirred overnight to give 2.83 g (R)-3-[1-(3-benzyloxypropyl)-7-cyanoindolin-5-yl]-2-methylpropionamide (V). To a soln. of 1.00 g V in 15 mL isopropanol was added 14 mL 15% aq. NaOCl at room temp., followed by adding 7 mL 2 M aq. NaOH under ice-cooling, and the resulting mixt. was stirred at 40° for 1 h to give 0.915 g (R)-5-(2-aminopropyl)-1-(3-benzyloxypropyl)indoline-7-carbonitrile (VI). To a soln. of 0.80 g VI in 8 mL tert-butanol were added 0.291 g Na2CO3 and 2-[2-(2,2,2-trifluoroethoxy)phenoxy]ethyl trifluoromethanesulfonate and refluxed overnight to give 0.564 g (R)-1-(3-benzyloxypropyl)-5-[2-[2-[2-(2,2,2-trifluoroethoxy)phenoxy]ethylamino]propyl]indoline-7-carbonitrile which (0.50 g) was dissolved in 5 mL MeCN, stirred at room temp. with 0.135 mL 30% aq. H2O2 and 0.054 mL 5 M aq. NaOH overnight and then with 0.100 mL 30% aq. H2O2 and 0.100 mL 5 M aq. NaOH for 5 h to give 0.391 g (R)-1-(3-benzyloxypropyl)-5-[2-[2-[2-(2,2,2-trifluoroethoxy)phenoxy]ethylamino]propyl]indoline-7-carboxamide (VII). A soln. of 0.35 g VII in 3 mL ethanol was treated with 1.44 mL 1 M aq. HCl and 0.060 g 10% Pd-C and stirred under hydrogen atm. for 3 h to give 0.207 g II.

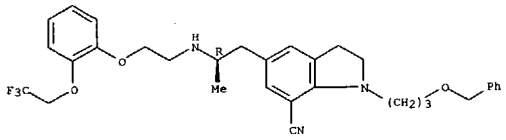
ACCESSION NUMBER: 2002:708796 CAPLUS
DOCUMENT NUMBER: 137:232552
TITLE: Preparation of 1-(3-benzyloxypropyl)-5-(2-substituted propyl)indolines as intermediates for drug for treating dysuria
INVENTOR(S): Yamaguchi, Toshiaki; Takeuchi, Hideki; Shiohara, Hiroaki
PATENT ASSIGNEE(S): Kissei Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002265444	A2	20020918	JP 2001-65686	20010308

PRIORITY APPLN. INFO.: JP 2001-65686 20010308
OTHER SOURCE(S): CASREACT 137:232552; MARPAT 137:232552
IT **459868-77-0P**, (R)-1-(3-Benzyloxypropyl)-5-[2-[[2-[2-(2,2,2-trifluoroethoxy)phenoxy]ethyl]amino]propyl]indoline-7-carbonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1-(3-benzyloxypropyl)-5-(2-substituted propyl)indolines as intermediates for drug for treating dysuria)
RN 459868-77-0 CAPLUS
CN 1H-Indole-7-carbonitrile, 2,3-dihydro-1-[3-(phenylmethoxy)propyl]-5-[(2R)-2-[[2-[2-(2,2,2-trifluoroethoxy)phenoxy]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 218 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L14 ANSWER 219 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
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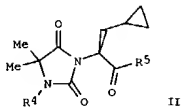


II

AB Title compds., e.g., R1NHCONHZCH2Z1CHRCONHCHR2CH2R3 [I; R = cyclopropylmethyl or CH2CHMe2; R1 = (2-methyl)phenyl; R2 = (un)substituted alkyl, -Ph, pyridinyl; R3 = CHO, CO2H, alkoxycarbonyl, CH2OR7, etc.; R7 = H or alkyl; Z = 2-hydroxy or -(fluoro)alkoxy-1,4-phenylene; Z1 = 5,5-di(trifluoro)methyl-2,4-dioxoimidazolidine-1,3-diyl] were prepared Thus, (S)-H2NCHRCO2CH2Ph (R = cyclopropylmethyl)(preparation given) was amidated by MeO2CNHCMe2CO2H and the produced cyclized to give dioxoimidazolidine II (R4 = H, R5 = OH) which was N-alkylated by 4-[3-(2-methylphenyl)uriedo]-3-methoxybenzyl chloride (preparation given) and the product amidated by (R)-H2NCHMeCH2CO2CMe3 to give, after saponification, II [R4 = 2-MeC6H4NHCONHZCH2, R5 = (R)-NHCHMeCH2CO2H, Z = 2-methoxy-1,4-phenylene]. Data for biol. activity of I were given.

ACCESSION NUMBER: 2002:695648 CAPLUS
DOCUMENT NUMBER: 137:216951
TITLE: Preparation of dioxoimidazolidinealkanoamides as VLA-4 receptor antagonists
INVENTOR(S): Wehner, Volkmar; Blum, Horst; Ruetten, Hartmut; Stilz, Hans Ulrich
PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany
SOURCE: Ger. Offen., 42 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10111877	A1	20020912	DE 2001-10111877	20010310
WO 2002072573	A1	20020919	WO 2002-EP1917	20020223

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

L14 ANSWER 219 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

EE 200300436	A	20031215	EE 2003-436	20020223
EP 1373249	A1	20040102	EP 2002-700268	20020223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003073723	A1	20030417	US 2002-92901	20020308
US 6680333	B2	20040120		
NO 2003003981	A	20030909	NO 2003-3981	20030909

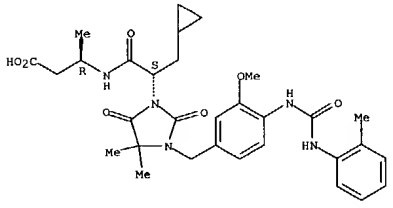
PRIORITY APPLN. INFO.: DE 2001-10111877 A 20010310
WO 2002-EP1917 W 20020223

OTHER SOURCE(S): MARPAT 137:216951

IT **457058-99-0P 457059-00-6P 457059-01-7P**
457059-02-8P 457059-03-9P 457059-04-0P
457059-05-1P 457059-06-2P 457059-17-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dioxoimidazolidinealkanoamides as VLA-4 receptor antagonists)

RN 457058-99-0 CAPLUS
CN Butanoic acid, 3-[[(2S)-3-cyclopropyl-2-[3-[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]methyl]-4,4-dimethyl-2,5-dioxo-1-imidazolidinyl]-1-oxopropyl]amino]-, (3R)- (9CI) (CA INDEX NAME)

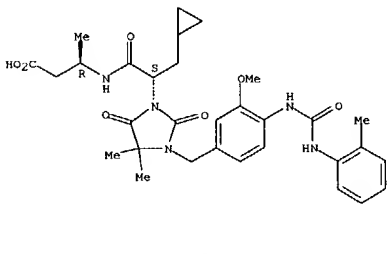
Absolute stereochemistry.



RN 457059-00-6 CAPLUS
CN Butanoic acid, 3-[[(2S)-3-cyclopropyl-2-[3-[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]methyl]-4,4-dimethyl-2,5-dioxo-1-imidazolidinyl]-1-oxopropyl]amino]-, monosodium salt, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

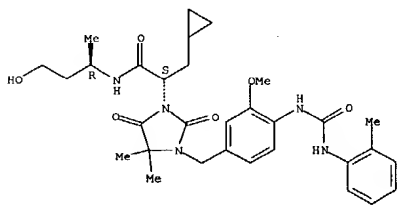
L14 ANSWER 219 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



● Na

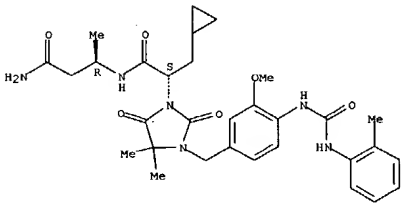
RN 457059-01-7 CAPLUS
CN 1-Imidazolidineacetamide, α-(cyclopropylmethyl)-N-[(1R)-3-hydroxy-1-methylpropyl]-3-[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]methyl]-4,4-dimethyl-2,5-dioxo-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



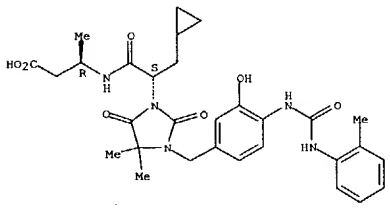
RN 457059-02-8 CAPLUS
CN 1-Imidazolidineacetamide, N-[(1R)-3-amino-1-methyl-3-oxopropyl]-α-(cyclopropylmethyl)-3-[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]methyl]-4,4-dimethyl-2,5-dioxo-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



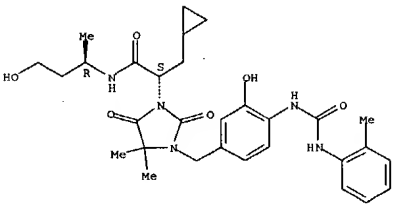
RN 457059-03-9 CAPLUS
CN Butanoic acid, 3-[[(2S)-3-cyclopropyl-2-[3-[[3-hydroxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]methyl]-4,4-dimethyl-2,5-dioxo-1-imidazolidinyl]-1-oxopropyl]amino]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



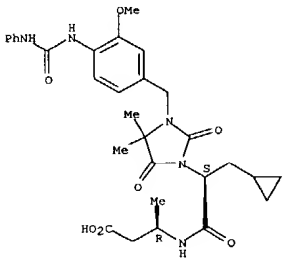
RN 457059-04-0 CAPLUS
CN 1-Imidazolidineacetamide, α-(cyclopropylmethyl)-3-[[3-hydroxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]methyl]-N-[(1R)-3-hydroxy-1-methylpropyl]-4,4-dimethyl-2,5-dioxo-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



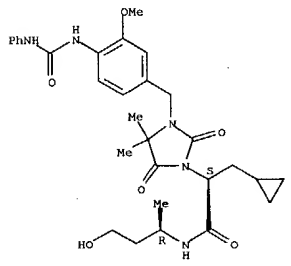
RN 457059-05-1 CAPLUS
CN Butanoic acid, 3-[[(2S)-3-cyclopropyl-2-[3-[[3-methoxy-4-[[(phenylamino)carbonyl]amino]phenyl]methyl]-4,4-dimethyl-2,5-dioxo-1-imidazolidinyl]-1-oxopropyl]amino]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



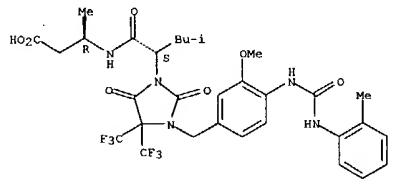
RN 457059-06-2 CAPLUS
CN 1-Imidazolidineacetamide, α-(cyclopropylmethyl)-N-[(1R)-3-hydroxy-1-methylpropyl]-3-[[3-methoxy-4-[[(phenylamino)carbonyl]amino]phenyl]methyl]-4,4-dimethyl-2,5-dioxo-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



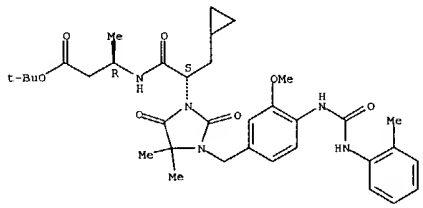
RN 457059-17-5 CAPLUS
CN Butanoic acid, 3-[[(2S)-2-[3-[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]methyl]-2,5-dioxo-4,4-bis(trifluoromethyl)-1-imidazolidinyl]-4-methyl-1-oxopentyl]amino]-, (3R)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **457059-23-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dioxoimidazolidinealkanoamides as VLA-4 receptor antagonists)
RN 457059-23-3 CAPLUS
CN Butanoic acid, 3-[[(2S)-3-cyclopropyl-2-[3-[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]methyl]-4,4-dimethyl-2,5-dioxo-1-imidazolidinyl]-1-oxopropyl]amino]-, 1,1-dimethylethyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 220 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

AB A symposium report. Conformation anal. of a β3-dodecapeptide was performed by two-dimensional homonuclear NMR spectroscopy in methanol and water.

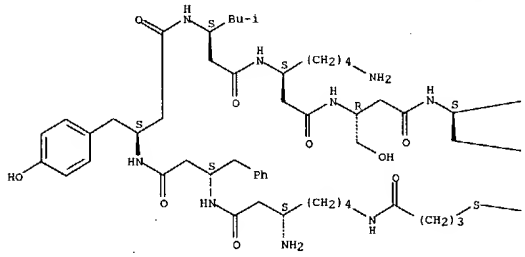
ACCESSION NUMBER: 2002:692364 CAPLUS
DOCUMENT NUMBER: 138:354198
TITLE: NMR structural investigation of a β3-dodecapeptide with proteinogenic side chains in MeOH and water
AUTHOR(S): Etezady-Esfarjani, Touraj; Hilty, Christian; Wuethrich, Kurt; Rueping, Magnus; Seebach, Dieter
CORPORATE SOURCE: Institut fuer Molekularbiologie und Biophysik, Eidgenoessiche Technische Hochschule, Zurich, CH-8093, Switz.
SOURCE: Peptides: The Wave of the Future, Proceedings of the Second International and the Seventeenth American Peptide Symposium, San Diego, CA, United States, June 9-14, 2001 (2001), 312-313. Editor(s): Lebl, Michal; Houghten, Richard A. American Peptide Society: San Diego, Calif.
CODEN: 69DBAL; ISBN: 0-9715560-0-8
DOCUMENT TYPE: Conference
LANGUAGE: English

IT **454486-18-1**
RL: PRP (Properties)
(conformations of a β-dodecapeptide in MeOH and water as analyzed by NMR spectroscopy)

RN 454486-18-1 CAPLUS
CN 5-Thia-3,10,18,22,26,30,34,38,42,46,50,54,58-tridecaazahenhexacontan-61-oic acid, 15-amino-31,39,55-tris(4-aminobutyl)-35,47-bis(hydroxymethyl)-23-[(4-hydroxyphenyl)methyl]-59-methyl-51-(1-methylethyl)-27-(2-methylpropyl)-2,9,17,21,25,29,33,37,41,45,49,53,57-tridecaoxo-19,43-bis(phenylmethyl)-, (15S,19S,23S,27S,31S,35R,39S,43S,47R,51R,55S,59S)- (9CI) (CA INDEX NAME)

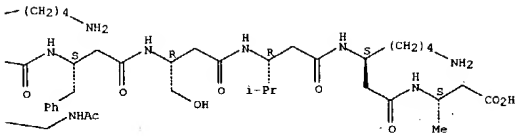
Absolute stereochemistry.

PAGE 1-A



L14 ANSWER 220 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-B



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 221 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

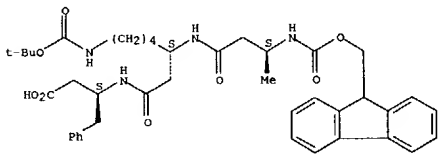
AB A symposium report. An improved synthetic methodol. for the solid-phase synthesis of long-chain β-peptides is described. The method was tested by synthesizing dodecapeptide and tetracosapeptide by coupling single amino acids and a series of homologous peptides by coupling β-peptidic triades. β-Tripeptide precursor Fmoc-(β-HAla-β-HLys(Boc)-β-HPhe)-OH was synthesized in eight steps from the corresponding α-amino acids with an overall yield of 60%.

ACCESSION NUMBER: 2002:692347 CAPLUS
DOCUMENT NUMBER: 138:321541
TITLE: Recent advances in the solid-phase synthesis of long-chain β-peptides
AUTHOR(S): Frackenpohl, Jens; Schreiber, Juerg V.; Arvidsson, Per I.; Seebach, Dieter
CORPORATE SOURCE: Laboratorium fuer Organische Chemie der Eidgenoessischen Technischen Hochschule, Zurich, CH-8092, Switz.
SOURCE: Peptides: The Wave of the Future, Proceedings of the Second International and the Seventeenth American Peptide Symposium, San Diego, CA, United States, June 9-14, 2001 (2001), 275-276. Editor(s): Lebl, Michal; Houghten, Richard A. American Peptide Society: San Diego, Calif.
CODEN: 69DBAL; ISBN: 0-9715560-0-8
DOCUMENT TYPE: Conference
LANGUAGE: English

IT **514223-57-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase synthesis of long-chain β-peptides)

RN 514223-57-5 CAPLUS
CN 14-Oxa-2,6,12-triazahexadecanoic acid, 7-[2-[[(1S)-1-(carboxymethyl)-2-phenylethyl]amino]-2-oxoethyl]-3,15,15-trimethyl-5,13-dioxo-, 1-(9H-fluoren-9-ylmethyl) ester, (3S,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 222 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

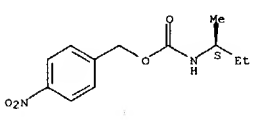
AB 1,2,4-Dithiazolidine-3,5-dione can be used as a nitrogen nucleophile in a modified Mitsunobu procedure to give N-alkylated products which can be converted via isocyanates, into amine derivs., under very mild conditions.
For example, the reaction of 1,2,4-dithiazolidine-3,5-dione with (2R)-2-butanol 2-[(1S)-1-methylpropyl]-1,2,4-dithiazolidine-3,5-dione (I) with inversion at the chiral center. Treatment of I with 4-nitrobenzenemethanol in the presence of triphenylphosphine/methylbenzene gave [(1S)-1-methylpropyl]carbamic acid 4-nitrophenyl ester via an intermediate isocyanate.

ACCESSION NUMBER: 2002:687922 CAPLUS
DOCUMENT NUMBER: 138:238082
TITLE: 1,2,4-Dithiazolidine-3,5-dione as an isocyanate equivalent in the Mitsunobu reaction
AUTHOR(S): Wood, Mark E.; Cane-Honeysett, Daniel J.; Dowle, Michael D.
CORPORATE SOURCE: School of Chemistry, University of Exeter, Exeter, EX4 4QD, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2002), (18), 2046-2047
CODEN: JCSPCE; ISSN: 1472-7781
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:238082

IT **501675-47-4P 501675-48-5P 501675-51-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(1,2,4-dithiazolidine-3,5-dione as isocyanate equivalent in Mitsunobu reaction of alcs.)

RN 501675-47-4 CAPLUS
CN Carbamic acid, [(1S)-1-methylpropyl]-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

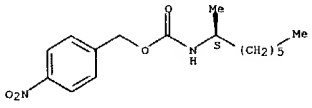
Absolute stereochemistry.



RN 501675-48-5 CAPLUS
CN Carbamic acid, [(1S)-1-methylheptyl]-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

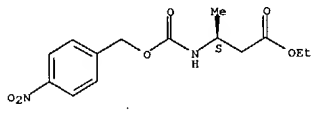
Absolute stereochemistry.

L14 ANSWER 222 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 501675-51-0 CAPLUS
CN Butanoic acid, 3-[[[(4-nitrophenyl)methoxy]carbonyl]amino]-, ethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L14 ANSWER 223 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
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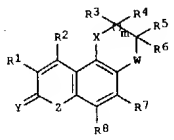

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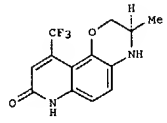


II

AB Title compds. I [R1 = H, F, Cl, Br, I, NO2, etc.; R2 = H, F, Cl, Br, I, CF3, CF2Cl, CF2H, etc.; R3-4 = H, alkoxy, SO0-2, amino, alkyl, haloalkyl, heteroalkyl, cycloalkyl, aryl, arylalkyl, heteroaryl, alkynyl, etc., or R3-4 taken together form a 3-8 membered (un)saturated (hetero)cyclic ring or R3, R5 taken together form a 3-8 membered (un)saturated ring or R3, R6 taken together form a 3-8 membered (un)saturated ring; R5-6 = H, CF3, CF2Cl, CF2H, CFH2, alkyl, haloalkyl, heteroalkyl, cycloalkyl, aryl, arylalkyl, heteroaryl, alkynyl, alkenyl, etc.; R7 = H, F, Cl, Br, I, alkyl, haloalkyl, heteroalkyl, aryl, heteroaryl, alkoxy, etc.; R8 = H, F, Cl, Br, I, alkyl, haloalkyl, heteroalkyl, aryl, heteroaryl, alkoxy, etc.; m = 0-2; W = O, SO0-2, N(H, alkyl, etc.,); X, Z = O, SO0-2, NH, etc.; Y = O, S, N(H, alkyl, etc.,), etc.] were prepared Over 50 synthetic examples were provided. For instance, 5-chloro-1,3-phenylenediamine was reacted with 4,4,4-trifluoroacetoacetate in EtOH at reflux for 18 h to give 5-Amino-7-chloro-3,4-dihydro-4-hydroxy-4-(trifluoromethyl)-1H-quinolin-2-one (37%). This was reduced (EtOH, KOAc, 10% Pd/C-H2, 2 h) to give 5-Amino-3,4-dihydro-4-hydroxy-4-(trifluoromethyl)-1H-quinolin-2-one (100%). This substrate was then subjected to the following reaction sequence: i. NaNO2/H2SO4; ii. EtOAc, i-PrNH2, NBS; iii. DMF, BnBr, CsF; iv. MsOH, HOAc; v. THF, NMM, Ph3P, DIAD, (R)-Boc-alinol; vi. CH2Cl2, TFA; vii. PhMe, Pd(O)Ligand, NaOBu-t; viii. HOAc, HCl, 90°, 4 h to give II. I are agonists, partial agonists and/or antagonists for androgen receptors (AR).

ACCESSION NUMBER: 2002:676021 CAPLUS
DOCUMENT NUMBER: 137:201318
TITLE: Preparation of tricyclic quinolinone androgen receptor modulator compounds
INVENTOR(S): Higuchi, Robert I.; Zhi, Lin; Karanewsky, Donald S.; Thompson, Anthony W.; Caferro, Thomas R.; Mani, Neelakandha S.; Chen, Jyun-Rung; Cummings, Marquis L.; Edwards, James P.; Adams, Mark E.; Deckhut, Charlotte L. F.
PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 142 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

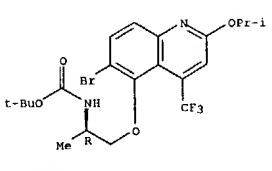
L14 ANSWER 223 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002068427	A1	20020906	WO 2002-IB538	20020223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002183314	A1	20021205	US 2002-80503	20020222
EP 1368357	A1	20031210	EP 2002-702590	20020223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.: US 2001-271115P P 20010223
WO 2002-IB538 W 20020223

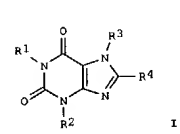
OTHER SOURCE(S): MARPAT 137:201318
IT **454169-38-1P**, (2R)-6-Bromo-5-[2-((tert-butoxycarbonyl)amino)propoxy]-2-isopropoxy-4-(trifluoromethyl)quinoline
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of tricyclic quinolinone androgen receptor modulator compds.)
RN 454169-38-1 CAPLUS
CN Carbamic acid, [(1R)-2-[[6-bromo-2-(1-methylethoxy)-4-(trifluoromethyl)-5-quinolinyl]oxy]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 224 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI



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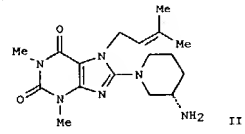


II

AB Xanthine derivs. of formula I [R1, R2 = H, alkyl, alkenyl, etc.; R3 = alkyl, arylalkyl, etc.; R4 = heterocyclyl, cycloalkyl, aminoalkyl, etc.] are prepared which exhibit an inhibitory effect on the activity of the dipeptidylpeptidase-IV enzyme. Pharmaceutical compns. containing I are described. Thus, II was prepared and had an IC50 of 22 nM against dipeptidylpeptidase-IV.

ACCESSION NUMBER: 2002:676018 CAPLUS
DOCUMENT NUMBER: 137:216824
TITLE: Preparation of xanthine derivatives as dipeptidylpeptidase-IV inhibitors
INVENTOR(S): Himmelsbach, Frank; Mark, Michael; Eckhardt, Matthias; Langkopf, Elke; Maier, Roland; Lotz, Ralf
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany
SOURCE: PCT Int. Appl., 373 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002068420	A1	20020906	WO 2002-EP1820	20020221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10109021	A1	20020905	DE 2001-10109021	20010224
DE 10117803	A1	20021024	DE 2001-10117803	20010410
DE 10140345	A1	20030227	DE 2001-10140345	20010817
DE 10203486	A1	20030731	DE 2002-10203486	20020130
EP 1368349	A1	20031210	EP 2002-701288	20020221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
EE 200300409	A	20031215	EE 2003-409	20020221
BR 2002007767	A	20040330	BR 2002-7767	20020221

L14 ANSWER 224 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

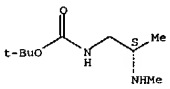
NO 2003003726	A	20030821	NO 2003-3726		20030821
US 2004077645	A1	20040422	US 2003-467961		20031205
PRIORITY APPLN. INFO.:			DE 2001-10109021	A	20010224
			DE 2001-10117803	A	20010410
			DE 2001-10140345	A	20010817
			DE 2002-10203486	A	20020130
			WO 2002-EP1820	W	20020221

OTHER SOURCE(S): MARPAT 137:216824

IT **454709-95-6P 454709-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of xanthine derivs. as dipeptidylpeptidase-IV inhibitors)

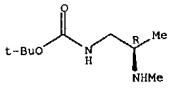
RN 454709-95-6 CAPLUS
CN Carbamic acid, [(2S)-2-(methylamino)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 454709-96-7 CAPLUS
CN Carbamic acid, [(2R)-2-(methylamino)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L14 ANSWER 225 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

AB Toward designing nonbiol. polymers that fold into predictable tertiary structures, we report a "β-oligomer" composed of β-amino acids that adopts a cooperatively folded structure. We have computationally designed a C2-sym. pair of interacting 14-helical β-oligomers stabilized via long-range interhelical interactions and stapled together by a disulfide bond. The reduced (BHBred) and oxidized (BHBox) forms of the synthetic β-oligomer represent the individual isolated helixes and the two-helix bundle, resp. We also prepared a third monomeric synthetic β-oligomer (BHBmon) to avoid inadvertent disulfide formation during characterization. CD spectroscopy revealed that BHBox showed a 2-fold increase in secondary structure, relative to the monohelical controls, BHBred and BHBmon. Further, BHBox showed a sigmoidal thermal unfolding curve with a per-residue van't Hoff enthalpy of approx. 0.7 kcal/(mol·residue), analogous to folded proteins. In contrast, BHBmon shows a broad thermal transition, typical of multistate unfolding for monomeric helixes. Also, anal. ultracentrifugation showed that BHBmon and BHBox were monomeric at concns. ≤800 and 280 μM, resp. Therefore, the enhanced helicity of BHBox could be attributed to intramol. helix-helix interactions.

ACCESSION NUMBER:	2002:675439 CAPLUS
DOCUMENT NUMBER:	137:348094
TITLE:	Long-Range Interactions Stabilize the Fold of a Non-natural Oligomer
AUTHOR(S):	Cheng, Richard P.; DeGrado, William F.
CORPORATE SOURCE:	Johnson Research Foundation, Department of Biochemistry and Biophysics, University of Pennsylvania School of Medicine, Philadelphia, PA, 19104-6059, USA
SOURCE:	Journal of the American Chemical Society (2002), 124(39), 11564-11565 CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER:	American Chemical Society
DOCUMENT TYPE:	Journal
LANGUAGE:	English

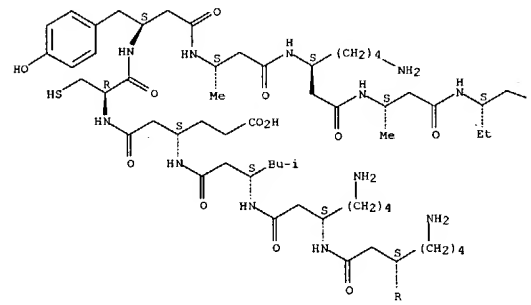
IT **474687-27-9 474687-28-0**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(long-range interactions stabilize fold of β-oligomer composed of β-amino acids)

RN 474687-27-9 CAPLUS
CN D-Aspartic acid, N3-[N3-[N3-[N3-L-cysteinyl-(3S)-3,7-diaminoheptanoyl-(3S)-3-aminobutanoyl-(3S)-3-aminopentanoyl-(3S)-3-amino-5-carboxypentanoyl-L-cysteinyl]-(3S)-3,7-diaminoheptanoyl]-(3S)-3,7-diaminoheptanoyl-(3S)-3-amino-5-methylhexanoyl-(3S)-3-amino-5-carboxypentanoyl-L-cysteinyl-(βS)-β-amino-4-hydroxybenzenebutanoyl-(3S)-3-aminobutanoyl]-(3S)-3,7-diaminoheptanoyl-(3S)-3-aminobutanoyl-(3S)-3-aminopentanoyl- (9CI) (CA INDEX NAME)

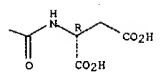
Absolute stereochemistry.

L14 ANSWER 225 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A

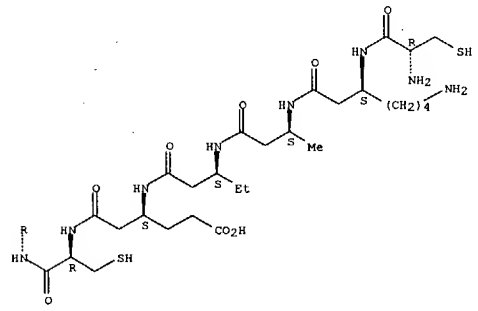


PAGE 1-B



L14 ANSWER 225 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 2-A

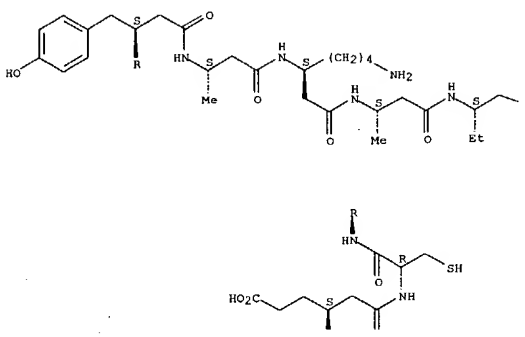


RN 474687-28-0 CAPLUS
CN D-Aspartic acid, N3-[N3-[N-[(3S)-5-carboxy-3-[[(3S)-3-[[(3S)-3-[[(3S)-3,7-diamino-1-oxoheptyl]amino]-1-oxobutyl]amino]-1-oxopentyl]amino]-1-oxopentyl]-L-cysteinyl]-(3S)-3,7-diaminoheptanoyl]-(3S)-3,7-diaminoheptanoyl-(3S)-3-amino-5-methylhexanoyl-(3S)-3-amino-5-carboxypentanoyl-L-cysteinyl-(βS)-β-amino-4-hydroxybenzenebutanoyl-(3S)-3-aminobutanoyl]-(3S)-3,7-diaminoheptanoyl-(3S)-3-aminobutanoyl-(3S)-3-aminopentanoyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 225 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



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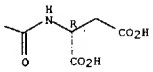
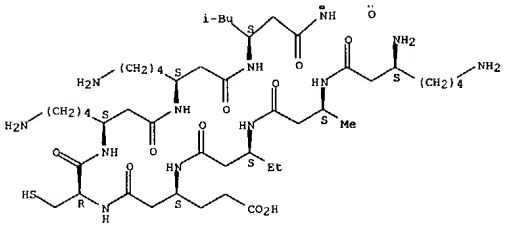


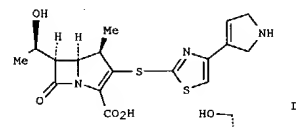
L14 ANSWER 225 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 2-A



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 226 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI



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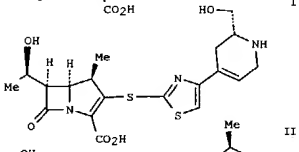
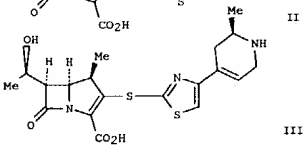


II



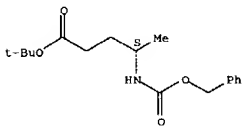
III

AB Discovery of novel antimicrobial agents effective against infections caused by drug-resistant pathogens is an important objective. In order to find a new parenteral carbapenem antibiotic, which has potent antibacterial activity especially against methicillin-resistant staphylococci, vancomycin-resistant enterococci and penicillin-resistant Streptococcus pneumoniae, a series of 1 β-methylcarbapenems with thiazol-2-ylthio groups at the C-2 position were synthesized. Structure-activity relationships were investigated which led to SM-197436 I, SM-232721 II and SM-232724 III, being selected for further evaluation.

ACCESSION NUMBER: 2002:674523 CAPLUS
DOCUMENT NUMBER: 137:369869
TITLE: New anti-MRSA and anti-VRE carbapenems; synthesis and structure-activity relationships of 1 β-methyl-2-(thiazol-2-ylthio)carbapenems
AUTHOR(S): Sunagawa, Makoto; Itoh, Masanori; Kubota, Katsumi; Sasaki, Akira; Ueda, Yutaka; Angehrn, Peter; Bourson, Anne; Goetschi, Erwin; Hebeisen, Paul; Then, Rudolf L.
CORPORATE SOURCE: Sumitomo Pharmaceuticals Research Division, Osaka, 554-0022, Japan
SOURCE: Journal of Antibiotics (2002), 55(8), 722-757
CODEN: JANTAJ; ISSN: 0021-8820

L14 ANSWER 226 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **475266-28-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1β-methyl-2-(thiazol-2-ylthio)carbapenems as new anti-MRSA and anti-VRE carbapenems antibacterials, and establishment of the structure activity relationship)
RN 475266-28-5 CAPLUS
CN Pentanoic acid, 4-[[(phenylmethoxy)carbonyl]amino]-, 1,1-dimethylethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 227 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

AB The equilibrium stability consts. (Ks) of ammonium pyrazolate complexes [L2-]2RN(R')H2+ (3, R' = H and 4, R' = Me) formed from a macrocyclic disodium dipyrazolate salt 2[L2-] 2Na+ and ammonium salts (RNH3+X- or RN(Me)H2+X-) of psychotropic drugs and neurotransmitter catecholamines have been evaluated by electrochem. methods in DMSO solution The resulting Ks values demonstrate that, except for (±)-amphetamine, the complexes formed by lipophilic primary [mescaline, (+)-amphetamine, (±)-p-methoxyamphetamine (PMA), (±)-3,4-methylenedioxyamphetamine (MDA)] and secondary [(±)-methamphetamine, (+)-methamphetamine and (±)-3,4-methylenedioxymethamphetamine (MDMA ecstasy')] phenethylamines are more stable than those formed from hydrophilic ones (dopamine and norepinephrine). A 1H and 13C NMR study on the formation of complexes of structure 3 and 4 formed from primary [mescaline, (+)-amphetamine] and secondary [(+)-methamphetamine] ammonium salts is given.

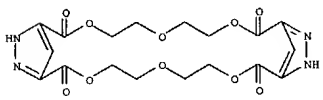
ACCESSION NUMBER: 2002:647697 CAPLUS
DOCUMENT NUMBER: 138:406723
TITLE: Effective complexation of psychotropic phenethylammonium salts from a disodium dipyrazolate salt of macrocyclic structure
AUTHOR(S): Reviriego, Felipe; Navarro, Pilar; Domenech, Antonio; Garcia-Espana, Enrique
CORPORATE SOURCE: Instituto de Quimica Medica, CSIC, Madrid, 28006, Spain
SOURCE: Journal of the Chemical Society, Perkin Transactions 2
(2002), (9), 1634-1638
CODEN: JCSPGI; ISSN: 1472-779X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **531513-34-5**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(complexation of psychotropic phenethylammonium salts from a disodium dipyrazolate salt of macrocyclic structure)

RN 531513-34-5 CAPLUS
CN 3,6,9,16,19,22-Hexaoxa-12,13,25,26-tetraazatricyclo[22.2.1.111,14]octacosa-1(27),11,14(28),24-tetraene-2,10,15,23-tetrone, compd. with (αS)-N,α-dimethylbenzeneethanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 134778-22-6
CMF C18 H20 N4 O10



L14 ANSWER 227 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CM 2

CRN 537-46-2
CMF C10 H15 N

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 228 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

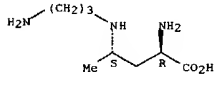
AB A versatile and efficient template synthesis has been developed to synthesize novel polyamines, such as isospermidine, via amino acids, such as (2R,4S/2S,4R)-N4-(3-aminopropyl)-2,4-diaminopentanoic acid, using cobalt(III) to assemble the three precursor components in a biomimetic manner.

ACCESSION NUMBER: 2002:647462 CAPLUS
DOCUMENT NUMBER: 138:187547
TITLE: Assembly of polyamines via amino acids from three components using cobalt(III) template methodology
AUTHOR(S): Laval, Gilles; Clegg, William; Crane, Christopher G.; Hammershoi, Anders; Sargeson, Alan M.; Golding, Bernard T.
CORPORATE SOURCE: Department of Chemistry, University of Newcastle upon Tyne, Newcastle upon Tyne, NE1 7RU, UK
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (17), 1874-1875
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:187547

IT **498579-34-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(assembly of polyamines via amino acids from three components using cobalt(III) template methodol.)

RN 498579-34-3 CAPLUS
CN D-Norvaline, 4-[(3-aminopropyl)amino]-, dihydrochloride, (4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

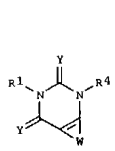


●2 HCl

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 229 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

GI



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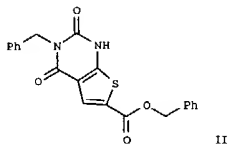


II

AB Title fused pyrimidinones I [wherein C2W = 5-membered (hetero)cyclic diradical substituted with ABR3 and optionally substituted with R2; A = CO or SO0-2; B = O or NR5; or AB = C.tplbond.C; R1, R4, and R5 = independently H, alkyl, alkenyl, alkynyl, (CH2)n-(hetero)aryl, (CH2)n-cycloalkyl, (CH2)n-heterocyclyl, or alkanoyl; R2 and R3 = independently H, alkyl, alkenyl, alkynyl CN, NO2, NR4R5, (CH2)n-cycloalkyl, or (CH2)n-(hetero)aryl; or R2 = halo; n = 0-5; or NR4R5 = (un)substituted heterocyclyl; with the proviso that R1 and R3 ≠ both H or alkyl; or pharmaceutically acceptable salts thereof] were prepared as matrix metalloproteinase (MMP) inhibitors, especially as selective MMP-13 inhibitors. For example, 3-benzyl-6-chloro-1H-pyrimidine-2,4-dione was coupled with mercaptoacetic acid Et ester using Na2CO3 in EtOH (67%) and the product cyclized with POCl3 in anhydrous DMF to give 3-benzyl-2,4-dioxo-1,2,3,4-tetrahydrothieno[2,3-d]pyrimidine-6-carboxylic acid Et ester (95%). Saponification (96%) followed by esterification with benzyl alc. and 1-cyclohexyl-3-(2-morpholinoethyl)carbodiimide metho-p-toluenesulfonate afforded II (12%). The latter selectively inhibited the hydrolytic activity of MMP-13 (0.61 μM) over MMP-1 (100 μM), MMP-2 (100 μM), MMP-3 (18 μM), MMP-7 (100 μM), MMP-9 (100 μM), MMP-12 (100 μM), and MMP-14 (100 μM) with the indicated IC50 values. I are useful for the treatment of diseases mediated by the MMP-13 enzyme, such as cancer, rheumatoid arthritis, or osteoarthritis (no data). Formulations of I are also disclosed.

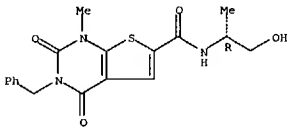
ACCESSION NUMBER: 2002:637683 CAPLUS
DOCUMENT NUMBER: 137:185504
TITLE: Preparation of thieno[2,3-d]pyrimidindiones as matrix metalloproteinase inhibitors for treatment of cancer, rheumatoid arthritis, and osteoarthritis
INVENTOR(S): Harter, William Glen; Li, Jie Jack; Ortwine, Daniel Fred; Shuler, Kevon Ray; Yue, Wen-song
PATENT ASSIGNEE(S): Warner-Lambert Company, USA
SOURCE: PCT Int. Appl., 278 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

L14 ANSWER 229 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002064598	A1	20020822	WO 2002-IB204	20020118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1370562	A1	20031217	EP 2002-711123	20020118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002007216	A	20040309	BR 2002-7216	20020118
US 2003004172	A1	20030102	US 2002-75073	20020213
PRIORITY APPLN. INFO.:			US 2001-268756P P	20010214
			WO 2002-IB204 W	20020118

OTHER SOURCE(S): MARPAT 137:185504
IT **448971-64-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(MMP inhibitor; preparation of thienopyrimidinediones as MMP inhibitors for
treatment of cancer, rheumatoid arthritis, and osteoarthritis)
RN 448971-64-0 CAPLUS
CN Thieno[2,3-d]pyrimidine-6-carboxamide, 1,2,3,4-tetrahydro-N-[(1R)-2-hydroxy-1-methylethyl]-1-methyl-2,4-dioxo-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

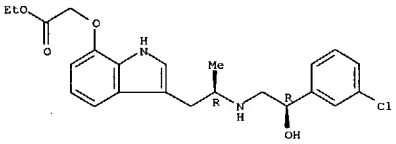
L14 ANSWER 230 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN.
AB Disclosed are a method of controlling the concentration of β3 adrenalin receptor in blood to thereby regulate the effect of blood insulin on the expression of the drug effect of a β3 adrenalin receptor agonist in case of administering the β3 adrenalin receptor agonist, and prepns. appropriate for controlling the β3 adrenalin receptor agonist concentration
in blood. Granules containing spheroidal crystalline cellulose 90, [3-[(2R)-[[(2R)-(3-Chlorophenyl)-2-hydroxyethyl]amino]propyl]-1H-indole-7-yloxy]acetate (I) 1, crystalline cellulose 4, hydroxypropyl cellulose 5 % was
coated with a coating solution containing methacrylic acid-Me methacrylate
copolymer (Eudragit S100) 100, tri-Et citrate 10, magnesium stearate 50 parts to obtain enteric granules. The obtained enteric granules showed controlled blood concentration of I in rats.
ACCESSION NUMBER: 2002:637517 CAPLUS
DOCUMENT NUMBER: 137:174951
TITLE: Pharmaceutical compositions providing controlled blood
concentration of β3 adrenalin receptor agonists
INVENTOR(S): Sugimoto, Tadanori; Furutani, Yasuji; Iwata, Motokazu;
Kuriyama, Teruaki; Higaki, Masaru; Kurita, Hideo
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002064133	A1	20020822	WO 2002-JP1223	20020214
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			JP 2001-40809 A	20010216

IT **448217-58-1**
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical compns. providing controlled blood concentration of β3
adrenalin receptor agonists)
RN 448217-58-1 CAPLUS
CN Acetic acid, [[3-[(2R)-2-[[(2R)-2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]-1H-indol-7-yl]oxy]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 230 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

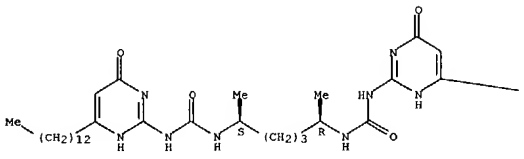


REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 231 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB Supramol. polymers, in which the monomer units are linked together by non-covalent interactions, provide unique opportunities to design responsive materials, as the system remains in constant equilibrium with its
environment. One of the most interesting aspects is the equilibrium between
linear and cyclic structures formed in solution and in bulk material, as this
strongly influences solution and material properties. Bifunctional mols. based on the strongly quadruple hydrogen bonding 2-ureido-4[1H]-pyrimidinone moiety form long supramol. polymers as well as small cyclic oligomers in solution The equilibrium between the different aggregates is
dependent on external conditions such as temperature, but also on the geometry
of the monomers. Here we report that small changes in the structure of the spacer between the hydrogen bonding units have a striking effect on the tendency of the mol. to form cyclic structures and, with that, on solution viscosity.
ACCESSION NUMBER: 2002:624907 CAPLUS
DOCUMENT NUMBER: 137:353337
TITLE: Tuning supramolecular ring-opening polymerization by conformational design
AUTHOR(S): ten Cate, A. Tessa; Sijbesma, Rint P.; Meijer, E. W.
CORPORATE SOURCE: Laboratory of Macromolecular and Organic Chemistry, Eindhoven University of Technology, Eindhoven, NL-5600
MB, Neth.
SOURCE: Polymer Preprints (American Chemical Society, Division
of Polymer Chemistry) (2002), 43(2), 333-334
CODEN: ACPPAY; ISSN: 0032-3934
PUBLISHER: American Chemical Society, Division of Polymer Chemistry
DOCUMENT TYPE: Journal; (computer optical disk)
LANGUAGE: English
IT **474901-70-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(effect of spacer structure on formation of cyclic structures and solution
viscosity)
RN 474901-70-7 CAPLUS
CN Urea, N,N''-[(1R,5S)-1,5-dimethyl-1,5-pentanediyl]bis[N'-(1,4-dihydro-4-oxo-6-tridecyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

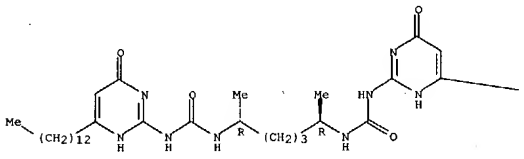


PAGE 1-B

IT **474901-71-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(effect of spacer structure on formation of cyclic structures and solution
viscosity)
RN 474901-71-8 CAPLUS
CN Urea, N,N''-[(1R,5R)-1,5-dimethyl-1,5-pentanediyl]bis[N'-(1,4-dihydro-4-oxo-6-tridecyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

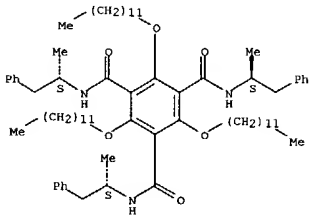


PAGE 1-B

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

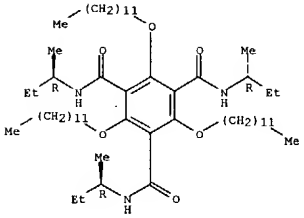
L14 ANSWER 232 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB Chiral side chains installed into the stacks of overcrowded arenes enforce
helical conformations . The assembly process can be directed with elec. fields as a result of a dipole moment parallel to the stacking direction. In concentrated solns., superhelices emerge that reflect circularly polarized
light.
ACCESSION NUMBER: 2002:623508 CAPLUS
DOCUMENT NUMBER: 138:4316
TITLE: The Consequences of chirality in crowded arenes-macromolecular helicity, hierarchical ordering,
and directed assembly
AUTHOR(S): Bushey, Mark L.; Hwang, Austin; Stephens, Peter W.; Nuckolls, Colin
CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027, USA
SOURCE: Angewandte Chemie, International Edition (2002), 41(15), 2828-2831
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:4316
IT **476684-22-7P 476684-26-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(consequences of chirality in crowded arenes-macromol. helicity hierarchical ordering and directed assembly)
RN 476684-22-7 CAPLUS
CN 1,3,5-Benzenetricarboxamide, 2,4,6-tris(dodecyloxy)-N,N',N''-tris[(1S)-1-methyl-2-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 476684-26-1 CAPLUS
CN 1,3,5-Benzenetricarboxamide, 2,4,6-tris(dodecyloxy)-N,N',N''-tris[(1R)-1-methylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 233 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

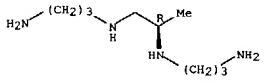
AB Syntheses of different open chain polyamines starting from enzymically prepared bis(amidoesters) are described. Some of these polyamines are also used as precursors in the syntheses of tetraazamacrocycles. This methodol. can also be applied to the synthesis of chiral compds.

ACCESSION NUMBER: 2002:619869 CAPLUS
DOCUMENT NUMBER: 138:14042
TITLE: Chemoenzymatic syntheses of polyamines and tetraazamacrocycles
AUTHOR(S): Rubio, Mercedes; Astorga, Covadonga; Alfonso, Ignacio; Rebolledo, Francisca; Gotor, Vicente
CORPORATE SOURCE: Departamento de Quimica Organica e Inorganica, Universidad de Oviedo, Oviedo, 33071, Spain
SOURCE: Synthetic Communications (2002), 32(16), 2441-2452
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:14042

IT **477808-30-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(chemoenzymic preparation of polyamines and tetraazamacrocycles)

RN 477808-30-3 CAPLUS
CN 1,2-Propanediamine, N,N'-bis(3-aminopropyl)-, tetrahydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

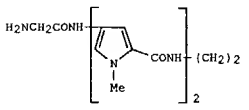


●4 HCl

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 234 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

GI



AB Compds. R1NH-Ar1-CO(NH-Ar2-CO)nNH-L-NH(CO-Ar3-NH)mCO-Ar4-NHR2 [R1, R2 = H, alkyl, (un)substituted alkanoyl or carbamoyl, at least one of which can form a salt; m, n = 0-4; Ar1-Ar4 = optionally substituted (hetero)arylene; L = alkylene which may be substituted by CONHR4, CONHNHR6, NHR9 (R4, R6, R9 = H, alkyl, aryl, etc.), or a guanidino group or L = (alkylene)x-Z-(alkylene)y-(Za)z, where x, y, and z = 0-2 and Z and Za = phenylene, cycloalkylene optionally fused to one or two phenylene ring(s), heterocyclene, O, S, NR10 (R10 = H, alkyl, cycloalkylamino, etc.), CONH or NHCO, provided that when Z and/or Za is NR10, it is separated from another nitrogen atom by at least two carbon atoms] or their pharmaceutically-acceptable salts were prepared as novel antibacterial/antifungal/antiparasit ic agents. Thus, compd I was prepared by a multistep sequence involving coupling reactions of Me 4-amino-1-methyl-1H-pyrrole-2-carboxylate, N-(tert-butoxycarbonyl)glycine pentafluorophenyl ester, and ethylenediamine. Compd I showed min. inhibitory concentration values >45.5 against various bacterial strains.

ACCESSION NUMBER: 2002:615567 CAPLUS
DOCUMENT NUMBER: 137:169795
TITLE: Preparation of polyamide analogs as antibacterial, antifungal, and antiparasitic agents
INVENTOR(S): Velligan, Mark D.; Khorlin, Alexander; Dyatkina, Natalia B.; Shi, Dong-Fang; Botyanszki, Janos; Liehr, Sebastian
PATENT ASSIGNEE(S): Genelabs Technologies, Inc., USA
SOURCE: PCT Int. Appl., 119 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002062755	A2	20020815	WO 2001-US45873	20011227
WO 2002062755	A3	20030821		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

L14 ANSWER 234 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

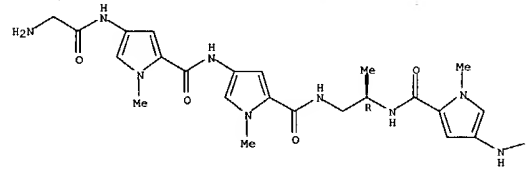
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
US 2002198254 A1 20021226 US 2001-26963 20011227
PRIORITY APPLN. INFO.: US 2000-258842P P 20001227
OTHER SOURCE(S): MARPAT 137:169795

IT **446882-00-4P 446882-02-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of polyamide analogs as antibacterial, antifungal, and antiparasitic agents)

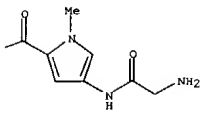
RN 446882-00-4 CAPLUS
CN 1H-Pyrrole-2-carboxamide, N,N'-[(1R)-1-methyl-1,2-ethanediyl]bis[4-[[[4-[(aminoacetyl)amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

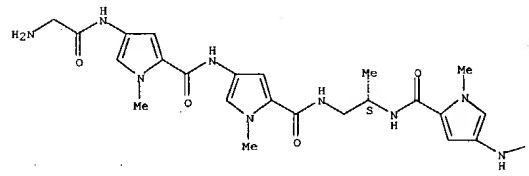


L14 ANSWER 234 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

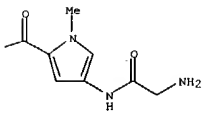
RN 446882-02-6 CAPLUS
CN 1H-Pyrrole-2-carboxamide, N,N'-[(1S)-1-methyl-1,2-ethanediyl]bis[4-[[[4-[(aminoacetyl)amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

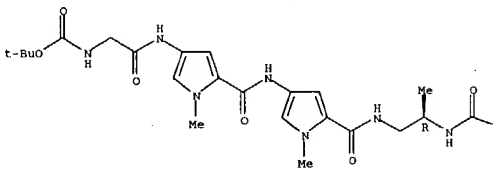


IT **446883-52-9P 446883-53-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of polyamide analogs as antibacterial, antifungal, and antiparasitic agents)

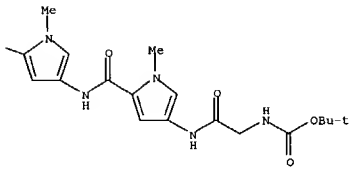
RN 446883-52-9 CAPLUS
CN Carbamic acid, [2-[[5-[[[5-[[[(1R)-2-[[[4-[[[4-[[[[(1,1-dimethylethoxy)carbonyl]amino]acetyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methylethyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



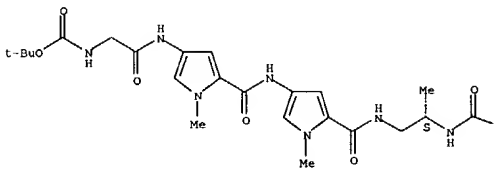
PAGE 1-B



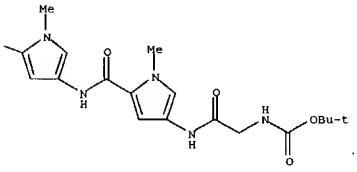
RN 446883-53-0 CAPLUS
CN Carbamic acid, [2-[[5-[[[5-[[[(1S)-2-[[[4-[[[4-[[[[(1,1-dimethylethoxy)carbonyl]amino]acetyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methylethyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



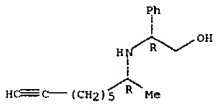
AB Propargylamines (R,R)-HOCH2CHPhNHCHRC.tplbond.C(CH2)4Me [R = Me, CHMe2, CH2CH2Ph], prepared in three steps from (R)-phenylglycinol, are readily isomerized at 0 °C with H2N(CH2)3NHK to form terminal acetylenic amines (R,R)-HOCH2CHPhNHCHR(CH2)5C.tplbond.CH, without any detectable epimerization of the chiral center, as already observed for propargyl alcs.
Enantiomerically pure (R)-H2NCHR(CH2)5C.tplbond.CH are obtained by oxidative cleavage of the chiral appendage.

ACCESSION NUMBER: 2002:603600 CAPLUS
DOCUMENT NUMBER: 138:72977
TITLE: Isomerization of chiral non-racemic α-substituted propargylic amines to terminal acetylenes
AUTHOR(S): Blanchet, Jerome; Bonin, Martine; Micouin, Laurent; Husson, Henri-Philippe
CORPORATE SOURCE: Laboratoire de Chimie Therapeutique associe au CNRS et
a l'Universite Rene Descartes (UMR 8638), Faculte des Sciences Pharmaceutiques et Biologiques, 4, av. l'Observatoire, Paris, 75270/06, Fr.
SOURCE: European Journal of Organic Chemistry (2002), (15), 2598-2602
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:72977

IT **481075-15-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(isomerization of chiral non-racemic α-substituted propargylic amines to terminal acetylenes)

RN 481075-15-4 CAPLUS
CN Benzeneethanol, β-[[(1R)-1-methyl-7-octynyl]amino]-, (βR)- (9CI) (CA INDEX NAME)

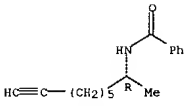
Absolute stereochemistry. Rotation (-).



IT **481075-21-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(isomerization of chiral non-racemic α-substituted propargylic amines to terminal acetylenes)

RN 481075-21-2 CAPLUS
CN Benzamide, N-[(1R)-1-methyl-7-octynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 236 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
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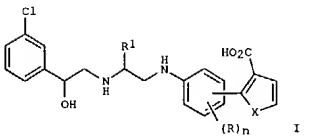
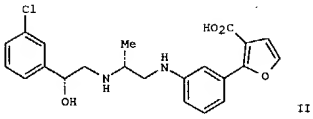


I



II

AB Title compds. I [X = O, X and where the heterocycle containing X is substituted meta or para to the depicted NH; R1 = H, alkyl; R = alkyl, halo, trifluoromethyl, alkoxy; n = 0-4] were prepared For instance, II was prepared in 3 steps. I are β-3 agonists and useful for treating beta-3 mediated diseases, e.g., diabetes or obesity.

ACCESSION NUMBER: 2002:594832 CAPLUS
DOCUMENT NUMBER: 137:154843
TITLE: Synthesis of aminoarylheterocyclic carboxylic acids as β-3 agonists used for obesity
INVENTOR(S): Deaton, David N.; Shearer, Barry George; Uehling, David Edward
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

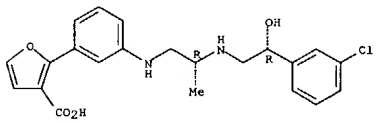
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002060885	A1	20020808	WO 2001-US49299	20011217

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

L14 ANSWER 236 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

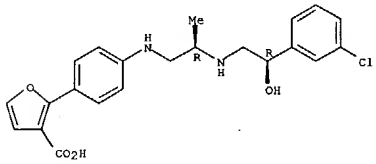
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
EP 1366033 A1 20031203 EP 2001-994312 20011217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
BR 2001016854 A 20040225 BR 2001-16854 20011217
NO 2003003401 A 20030930 NO 2003-3401 20030730
PRIORITY APPLN. INFO.: GB 2001-2408 A 20010131
WO 2001-US49299 W 20011217
OTHER SOURCE(S): MARPAT 137:154843
IT **445307-54-0P 445307-56-2P 445307-57-3P 445307-59-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug; synthesis of aminoarylheterocyclic carboxylic acids as β-3 agonists used for obesity)
RN 445307-54-0 CAPLUS
CN 3-Furancarboxylic acid, 2-[3-[[(2R)-2-[[(2R)-2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]amino]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 445307-56-2 CAPLUS
CN 3-Furancarboxylic acid, 2-[4-[[(2R)-2-[[(2R)-2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]amino]phenyl]- (9CI) (CA INDEX NAME)

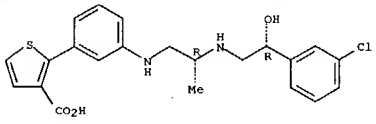
Absolute stereochemistry.



RN 445307-57-3 CAPLUS
CN 3-Thiophenecarboxylic acid, 2-[3-[[(2R)-2-[[(2R)-2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]amino]phenyl]- (9CI) (CA INDEX NAME)

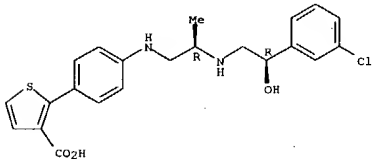
Absolute stereochemistry.

L14 ANSWER 236 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



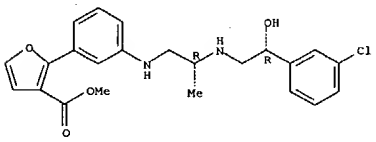
RN 445307-59-5 CAPLUS
CN 3-Thiophenecarboxylic acid, 2-[4-[[(2R)-2-[[(2R)-2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]amino]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



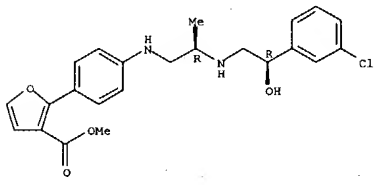
IT **445307-43-7P 445307-45-9P 445307-46-0P 445307-48-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; synthesis of aminoarylheterocyclic carboxylic acids as β-3 agonists used for obesity)
RN 445307-43-7 CAPLUS
CN 3-Furancarboxylic acid, 2-[3-[[(2R)-2-[[(2R)-2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]amino]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



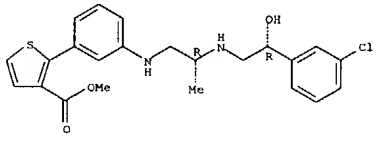
RN 445307-45-9 CAPLUS
CN 3-Furancarboxylic acid, 2-[4-[[(2R)-2-[[(2R)-2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]amino]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

L14 ANSWER 236 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Absolute stereochemistry.



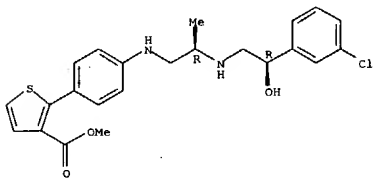
RN 445307-46-0 CAPLUS
CN 3-Thiophenecarboxylic acid, 2-[3-[[(2R)-2-[[(2R)-2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]amino]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 445307-48-2 CAPLUS
CN 3-Thiophenecarboxylic acid, 2-[4-[[(2R)-2-[[(2R)-2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]amino]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

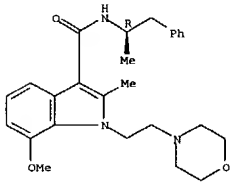


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS

L14 ANSWER 236 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 237 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB C-3 Amido-indoles were found to selectively bind to the CB2 receptor. Structure-activity structure-activity relationship (SAR) studies led to optimized compds. with excellent in vivo potency against LPS induced TNF-α release in murine models of cytokine production
ACCESSION NUMBER: 2002:585100 CAPLUS
DOCUMENT NUMBER: 138:231273
TITLE: C-3 Amido-Indole cannabinoid receptor modulators
AUTHOR(S): Hynes, John; Leftheris, Katerina; Wu, Hong; Pandit, Chennagiri; Chen, Ping; Norris, Derek J.; Chen, Bang-Chi; Zhao, Rulin; Kiener, Peter A.; Chen, Xiaorong; Turk, Lori A.; Patil-Koota, Vina; Gillooly, Kathleen M.; Shuster, David J.; McIntyre, Kim W.
CORPORATE SOURCE: Discovery Chemistry, Bristol-Myers Squibb, Princeton, NJ, 08543-4000, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(17), 2399-2402
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:231273
IT **501927-07-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(structure-activity relationship of amido-indoles as cannabinoid receptor modulators)
RN 501927-07-7 CAPLUS
CN 1H-Indole-3-carboxamide, 7-methoxy-2-methyl-N-[(1R)-1-methyl-2-phenylethyl]-1-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)

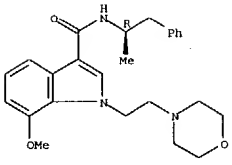
Absolute stereochemistry.



IT **501926-84-7**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(structure-activity relationship of amido-indoles as cannabinoid receptor modulators)
RN 501926-84-7 CAPLUS
CN 1H-Indole-3-carboxamide, 7-methoxy-N-[(1R)-1-methyl-2-phenylethyl]-1-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

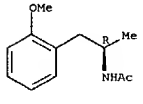
L14 ANSWER 237 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

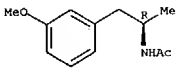
L14 ANSWER 238 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB Some pharmacol. active amines such as amphetamine, the isomeric o-, m- and
p-methoxyamphetamines, 4-phenylbutan-2-amine and mexiletine, as well as their corresponding acetamides, have been prepared in high yields and with
very high enantiomeric excesses. The method consists of the Candida antarctica lipase B (CAL-B)-mediated enantioselective acetylation of racemic amines using Et acetate as solvent and acyl donor. The enzyme follows Kazlauskas' rule with all amines, (R)-amides being obtained as the
major enantiomer in all cases. From the conversion values measured for both enantiomers, it can be deduced that the size of the substituents attached to the stereocenter is responsible for the enantioselectivity and
rate of some of these reactions.
ACCESSION NUMBER: 2002:585043 CAPLUS
DOCUMENT NUMBER: 138:89529
TITLE: CAL-B-catalyzed resolution of some pharmacologically interesting β-substituted isopropylamines
AUTHOR(S): Gonzalez-Sabin, Javier; Gotor, Vicente; Rebolledo, Francisca
CORPORATE SOURCE: Departamento de Quimica Organica e Inorganica, Universidad de Oviedo, Oviedo, 33071, Spain
SOURCE: Tetrahedron: Asymmetry (2002), 13(12), 1315-1320
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:89529
IT **484033-26-3P 484033-29-6P**
RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(CAL-B-catalyzed resolution of some pharmacol. interesting β-substituted isopropylamines)
RN 484033-26-3 CAPLUS
CN Acetamide, N-[(1R)-2-(2-methoxyphenyl)-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 484033-29-6 CAPLUS
CN Acetamide, N-[(1R)-2-(3-methoxyphenyl)-1-methylethyl]- (9CI) (CA INDEX NAME)

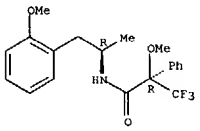
Absolute stereochemistry. Rotation (+).



IT **484033-36-5P 484033-38-7P 484033-40-1P**
484033-42-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(CAL-B-catalyzed resolution of some pharmacol. interesting β-substituted isopropylamines)

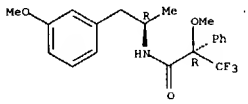
RN 484033-36-5 CAPLUS
CN Benzeneacetamide, α-methoxy-N-[(1R)-2-(2-methoxyphenyl)-1-methylethyl]-α-(trifluoromethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



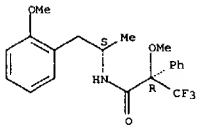
RN 484033-38-7 CAPLUS
CN Benzeneacetamide, α-methoxy-N-[(1R)-2-(3-methoxyphenyl)-1-methylethyl]-α-(trifluoromethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



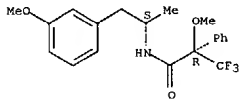
RN 484033-40-1 CAPLUS
CN Benzeneacetamide, α-methoxy-N-[(1S)-2-(2-methoxyphenyl)-1-methylethyl]-α-(trifluoromethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

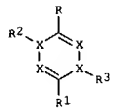


RN 484033-42-3 CAPLUS
CN Benzeneacetamide, α-methoxy-N-[(1S)-2-(3-methoxyphenyl)-1-methylethyl]-α-(trifluoromethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT



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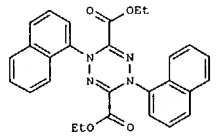


II

AB Disclosed are heterocyclic compds. and methods for their manufacture In particular, the compds. disclosed are represented by structure I [each X =
(independently) CH or N; R = alkoxy, alkyl, haloalkoxy, alkylketo, alkylthioketo, CO2H, CONR6R7, ester, thioester, reversed ester, reversed thioester, reversed amide, or COR4; R1 = same groups, except COR5 instead of COR4; R2, R3 = (un)substituted Ph, CH2Ph, α/β-naphthyl, CH2-α/β-naphthyl, certain N/O/S-heteroaryl or CH2-N/O/S-heteroaryl, terpenes, etc.; R4, R5 = methoxy, ethoxy, propoxy, Me, amino, methylamino, ethylamino, ethylamino, butylamino, piperidino, (R)-2-hydroxy-1-methylethylamino or enantiomer, (+)-isopinocampheylamino or enantiomer; R6, R7 = H, alkyl, or carbalkoxyalkyl; including physiol. acceptable salts, diastereomers, enantiomers, double-bond isomers, and/or mixts.]. Also disclosed are methods of using the disclosed compds., including use of the disclosed compds. to stimulate a cannabinoid receptor, to provide a physiol. effect in an animal or individual and to treat a condition in an animal or individual. Compds. I are surprisingly potent and selective cannabinoids. A table of 25 specific compds. is given, and the same compds. are covered individually by claims. A preparatory scheme is also covered by claims. For instance, reaction of 1-naphthalenediazonium sulfuric acid salt with Et 2-chloroacetoacetate gave 1-ClOH7-NHN:C(Cl)CO2Et. This ester was cyclodimerized by NaN(SiMe3)2 in THF at -78°, giving the invention tetrazine II. A representative compound I inhibited adenylate cyclase in an intracellular cAMP bioassay, indicating CB2 agonist activity. In binding studies using rat brain CB1 receptors and mouse spleen CB2 receptors, I generally showed selectivity for CB2 receptors, with II showing the highest selectivity (524-fold for CB2 over CB1).

ACCESSION NUMBER: 2002:574870 CAPLUS
DOCUMENT NUMBER: 137:140538
TITLE: Novel cannabimimetic ligands, particularly 1,2,4,5-tetrazine derivatives and analogs, and their preparation and pharmaceutical use as selective CB2 ligands
INVENTOR(S): Makriyannis, Alexandros; Deng, Hongfeng
PATENT ASSIGNEE(S): University of Connecticut, USA
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002058636	A2	20020801	WO 2002-US2157	20020125
WO 2002058636	A3	20021010		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1361876	A2	20031119	EP 2002-707564	20020125

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

US 2004077649	A1	20040422	US 2003-466403	20031031

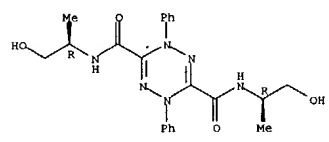
PRIORITY APPLN. INFO.: US 2001-264385P P 20010126
WO 2002-US2157 W 20020125

OTHER SOURCE(S): MARPAT 137:140538

IT **444683-37-8P**, N,N'-Di(β-hydroxy-α-(R)-methylethyl]-1,4-diphenyl-1,4-dihydro-1,2,4,5-tetrazine-3,6-dicarboxylic diamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of tetrazine derivs. and analogs as selective CB2 cannabimimetic ligands)

RN 444683-37-8 CAPLUS
CN 1,2,4,5-Tetrazine-3,6-dicarboxamide, 1,4-dihydro-N,N'-bis[(1R)-2-hydroxy-1-methylethyl]-1,4-diphenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 240 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

AB Five β-peptide thioesters containing 3, 4, 10 residues, e. g., NH2β3HPhe-β3HTyr-β3HLys-SEt, were prepared by manual solid-phase synthesis and purified by reverse-phase preparative HPLC. A β-undecapeptide and an α-undecapeptide with N-terminal β3-HCys and Cys residues were prepared by manual and machine synthesis, resp. Coupling of the thioesters with the cysteine derivs. in the presence of PhSH in aqueous solution occurred smoothly and quant. Pentadeca- and heneicosapeptides were isolated, after preparative RP-HPLC purification, in yields of up to 60%. Thus, the so-called native chemical ligation works well with β-peptides, producing larger β3- and α/β3-mixed peptides. All prepared compds. were characterized by high-resolution mass spectrometry (HR-MS) and by CD spectroscopy, including temperature and concentration dependence. β-Peptide with 21 residues shows an intense neg. Cotton effect near 210 nm but no zero-crossing above 190 nm, which is characteristic of β-peptidic 314-helical structures. Comparison of the CD spectra of the mixed α/β-pentadecapeptide NH2β3HAla-β3HPhe-β3HTyr-β3HGly-Cys-Gly-Ala-Asp-Tyr-Lys-(Asp)4-Lys-OH and a helical α-peptide indicate the presence of an α-peptidic 3.613 helix.

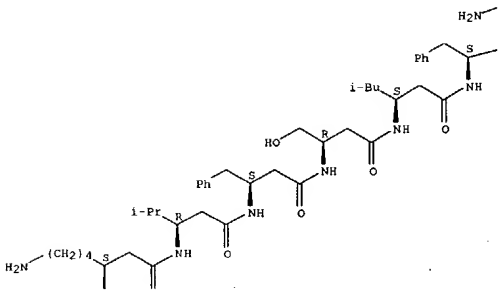
ACCESSION NUMBER: 2002:537111 CAPLUS
DOCUMENT NUMBER: 137:295232
TITLE: Synthesis of β3-peptides and mixed α/β3-peptides by thioligation
AUTHOR(S): Kimmerlin, Thierry; Seebach, Dieter; Hilvert, Donald
CORPORATE SOURCE: Laboratorium fur Organische Chemie der Eidgenossischen Technischen Hochschule, ETH-Honggerberg, Zurich, CH-8093, Switz.
SOURCE: Helvetica Chimica Acta (2002), 85(6), 1812-1826
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **470461-67-7P 470461-69-9P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase synthesis of β-peptide and mixed α/β-peptide derivs. by thioligation of peptide thioesters with α- or β- peptides cysteine peptides)

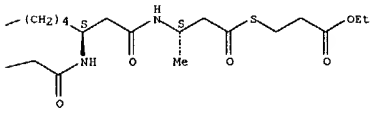
RN 470461-67-7 CAPLUS
CN 4-Thia-8,12,16,20,24,28,32,36,40-nonaazatetratetracontanoic acid, 43-amino-11,35-bis(4-aminobutyl)-39-[(1R)-1-hydroxyethyl]-23-(hydroxymethyl)-7-methyl-31-(1-methylethyl)-19-(2-methylpropyl)-5,9,13,17,21,25,29,33,37,41-decaoxo-15,27-bis(phenylmethyl)-, ethyl ester, (7S,11S,15S,19S,23R,27S,31R,35S,39R,43S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

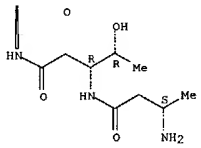
PAGE 1-A



PAGE 1-B



PAGE 2-A



RN 470461-69-9 CAPLUS

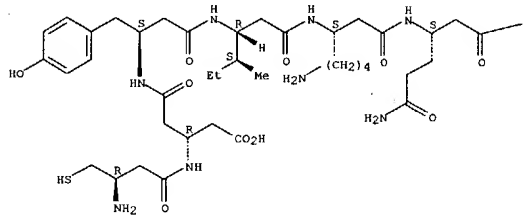
CN 2-Pyrrolidineacetic acid, 1-[(3S,7R,11S,15S,19S,23S,27R,31S,35R,39R)-39-amino-23-(4-aminobutyl)-19-(3-amino-3-oxopropyl)-35-(carboxymethyl)-7-(hydroxymethyl)-31-[(4-hydroxyphenyl)methyl]-40-mercapto-11-methyl-27-[(1S)-1-methylpropyl]-15-(2-methylpropyl)-1,5,9,13,17,21,25,29,33,37-decaoxo-3-(phenylmethyl)-4,8,12,16,20,24,28,32,36-nonaazatetracont-1-yl]-, (2S)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

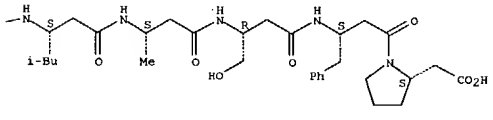
CRN 470461-68-8
CMF C70 H111 N13 O17 S

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CM 2

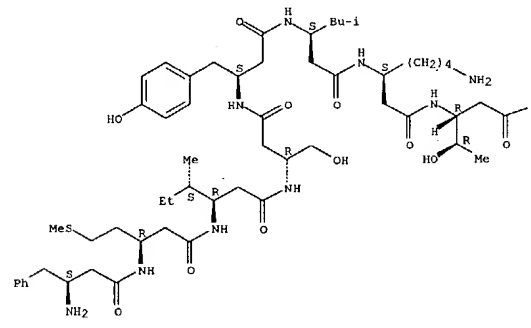
CRN 76-05-1
CMF C2 H F3 O2

IT **470461-66-6P 470461-72-4P 470461-74-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of β-peptide and mixed α/β-peptide derivs. by thioligation of peptide thioesters with α- or β- peptides cysteine peptides)

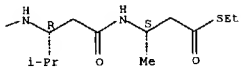
RN 470461-66-6 CAPLUS
CN 4,8,12,16,20,24,28,32,36-Nonaazatetracontanethioic acid, 39-amino-15-(4-aminobutyl)-11-[(1R)-1-hydroxyethyl]-27-(hydroxymethyl)-23-[(4-hydroxyphenyl)methyl]-3-methyl-7-(1-methylethyl)-31-[(1S)-1-methylpropyl]-19-(2-methylpropyl)-35-[2-(methylthio)ethyl]-5,9,13,17,21,25,29,33,37-nonaoxo-40-phenyl-, S-ethyl ester, (3S,7R,11R,15S,19S,23S,27R,31R,35R,39S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RN 470461-72-4 CAPLUS
CN 2-Pyrrolidineacetic acid,
1-[(3S,7R,11S,15S,19S,23S,27R,31S,35R,39R,47S,51
S,55S)-55-amino-23-(4-aminobutyl)-19-(3-amino-3-oxopropyl)-35-
(carboxymethyl)-7-(hydroxymethyl)-31,47-bis[(4-hydroxyphenyl)methyl]-39-
(mercaptomethyl)-11-methyl-27-[(1S)-1-methylpropyl]-15-(2-methylpropyl)-

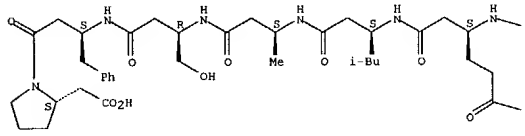
1,5,9,13,17,21,25,29,33,37,41,45,49,53-tetradecaoxo-3,51-bis(phenylmethyl)-
4,8,12,16,20,24,28,32,36,40,44,48,52-tridecaazahexapentacont-1-yl]-,
(2S)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

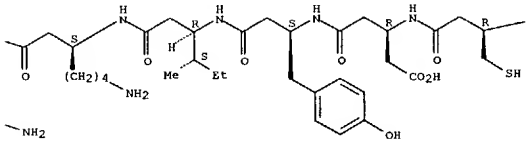
CRN 470461-71-3
CMF C97 H145 N17 O22 S

Absolute stereochemistry.

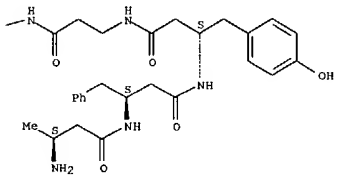
PAGE 1-A



PAGE 1-B



PAGE 1-C



CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 470461-74-6 CAPLUS
CN 2-Pyrrolidineacetic acid,
1-[(3S,7R,11S,15S,19S,23S,27R,31S,35R,39R,43S,47

S,51S,55S,59R,63S,67R,71S,75R,79S)-79-amino-23,47,71-tris(4-aminobutyl)-19-
(3-amino-3-oxopropyl)-35-(carboxymethyl)-75-[(1R)-1-hydroxyethyl]-7,59-

bis(hydroxymethyl)-31-[(4-hydroxyphenyl)methyl]-39-(mercaptomethyl)-11,43-
dimethyl-67-(1-methylethyl)-27-[(1S)-1-methylpropyl]-15,55-bis(2-
methylpropyl)-1,5,9,13,17,21,25,29,33,37,41,45,49,53,57,61,65,69,73,77-

eicosaoxo-3,51,63-tris(phenylmethyl)-4,8,12,16,20,24,28,32,36,40,44,48,52,

56,60,64,68,72,76-nonadecaazaoctacont-1-yl]-, (2S)-, trifluoroacetate
(salt) (9CI) (CA INDEX NAME)

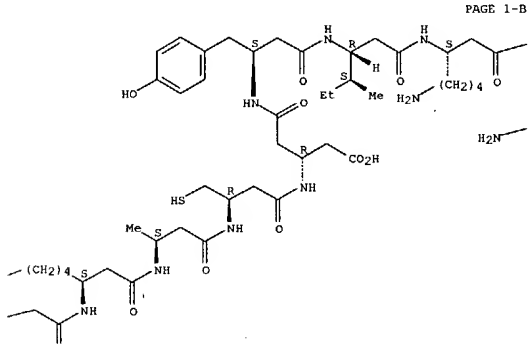
CM 1

CRN 470461-73-5
CMF C134 H215 N25 O29 S

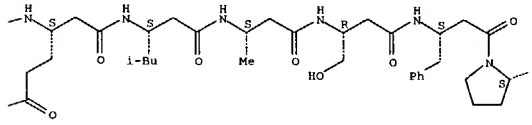
Absolute stereochemistry.

PAGE 1-A

PAGE 1-B



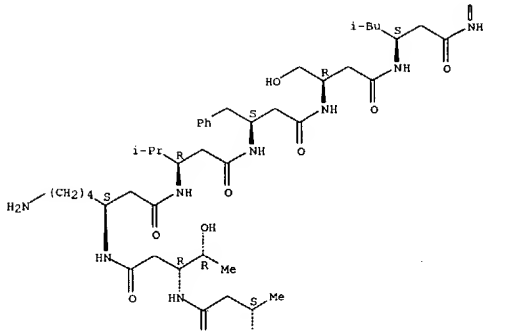
PAGE 1-C



PAGE 1-D

L14 ANSWER 240 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 2-A



PAGE 2-B

PAGE 3-A

CM 2

CRN 76-05-1
CMF C2 H F3 O2

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 241 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

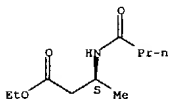
AB The Candida antarctica lipase B-catalyzed reactions of five β-amino esters with neat Bu butanoate and with 2,2,2-trifluoroethyl butanoate in diisopropyl ether were studied, as were the reactions of the same β-amino esters and their N-butanamides with neat butanol. The possibility for sequential resolution, where the amino and ester functions of the substrate both react with an achiral butanoate, became less likely with increasing size of the substrate from Et 3-aminobutanoate to pentanoate or larger. On the other hand, the alcoholizes of N-acylated β-amino esters successfully proceeded in butanol with E>100. Gram-scale resolution of the N-butanoylated was performed to demonstrate the usefulness of the method.

ACCESSION NUMBER: 2002:523211 CAPLUS
DOCUMENT NUMBER: 137:310500
TITLE: Structural effects on chemo- and enantioselectivity of Candida antarctica lipase B - resolution of β-amino esters
AUTHOR(S): Gedey, Szilvia; Liljeblad, Arto; Lazar, Laszlo; Fulop, Ferenc; Kanerva, Liisa T.
CORPORATE SOURCE: Laboratory of Synthetic Drug Chemistry and Department of Chemistry, University of Turku, Turku, FIN-20520, Finland
SOURCE: Canadian Journal of Chemistry (2002), 80(6), 565-570
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **470707-07-4P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(structural effects on chemo and enantioselectivity of Candida antarctica lipase B and resolution of β-amino esters)

RN 470707-07-4 CAPLUS
CN Butanoic acid, 3-[(1-oxobutyl)amino]-, ethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 242 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

AB The importance of hydrogen bonding in β-peptide 314-helixes is demonstrated by an NMR anal. of three β-heptadepsipeptides containing a 3-hydroxybutanoic residue in position 2, 4 or 6.

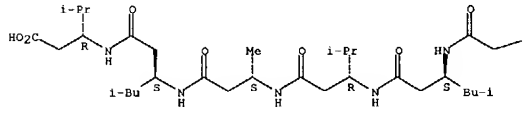
ACCESSION NUMBER: 2002:517314 CAPLUS
DOCUMENT NUMBER: 138:39521
TITLE: β-Depsipeptides - the effect of a missing and a weakened hydrogen bond on the stability of the β-peptidic 314-helix
AUTHOR(S): Seebach, Dieter; Mahajan, Yogesh R.; Senthilkumar, Ramanathan; Rueping, Magnus; Jaun, Bernhard
CORPORATE SOURCE: Laboratorium fuer Organische Chemie der Eidgenoessischen Technischen Hochschule, ETH-Honggerberg, Zurich, CH-8093, Switz.
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (15), 1598-1599
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:39521

IT **478867-08-2P 478867-09-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(hydrogen bonding in β-peptide 314-helixes by NMR of β-heptadepsipeptides containing hydroxybutanoic residue)

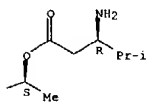
RN 478867-08-2 CAPLUS
CN 24-Oxa-4,8,12,16,20-pentaazanonacosanoic acid, 27-amino-11,23,28-trimethyl-3,15-bis(1-methylethyl)-7,19-bis(2-methylpropyl)-5,9,13,17,21,25-hexaoxo-, (3R,7S,11S,15R,19S,23S,27R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

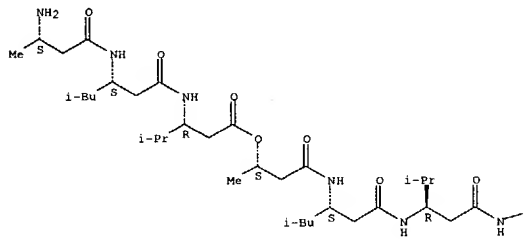


RN 478867-09-3 CAPLUS

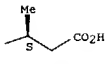
L14 ANSWER 242 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 16-Oxa-4,8,12,20,24-pentaazaoctacosanoic acid,
27-amino-3,15-dimethyl-7,19-
bis(1-methylethyl)-11,23-bis(2-methylpropyl)-5,9,13,17,21,25-hexaoxo-,
(3S,7R,11S,15S,19R,23S,27S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

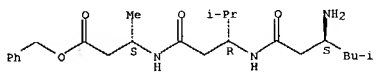


IT **478867-11-7 478867-12-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogen bonding in β-peptide 314-helixes by NMR of
β-heptadepsipeptides containing hydroxybutanoic residue)
RN 478867-11-7 CAPLUS
CN Hexanoic acid,
5-methyl-3-[[(3S)-1-oxo-3-[[(phenylmethoxy)carbonyl]amino]b
utyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

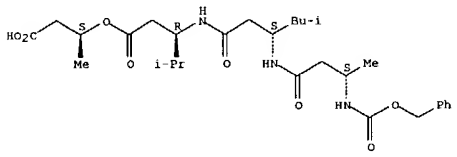
L14 ANSWER 242 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
methyl-1-oxopentyl]amino]-, phenylmethyl ester, (3S)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



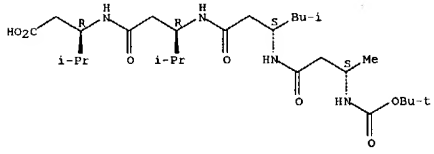
RN 478867-23-1 CAPLUS
CN 14-Oxa-2,6,10-triazaheptadecanedioic acid, 3,15-dimethyl-11-(1-
methylethyl)-7-(2-methylpropyl)-5,9,13-trioxo-, 1-(phenylmethyl) ester,
(3S,7S,11R,15S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



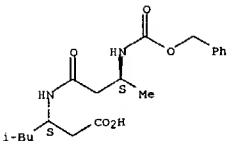
RN 478867-28-6 CAPLUS
CN 2,6,10,14-Tetraazaheptadecanedioic acid,
3-methyl-11,15-bis(1-methylethyl)-
7-(2-methylpropyl)-5,9,13-trioxo-, 1-(1,1-dimethylethyl) ester,
(3S,7S,11R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



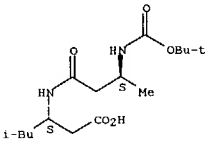
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 242 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



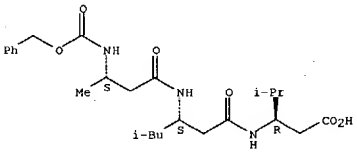
RN 478867-12-8 CAPLUS
CN Hexanoic acid, 3-[[(3S)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-
oxobutyl]amino]-5-methyl-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **478867-19-5P 478867-21-9P 478867-23-1P**
478867-28-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(hydrogen bonding in β-peptide 314-helixes by NMR of
β-heptadepsipeptides containing hydroxybutanoic residue)
RN 478867-19-5 CAPLUS
CN 2-Oxa-4,8,12-triazapentadecan-15-oic acid, 5-methyl-13-(1-methylethyl)-9-
(2-methylpropyl)-3,7,11-trioxo-1-phenyl-, (5S,9S,13R)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



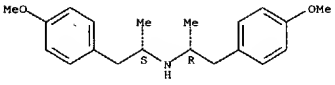
RN 478867-21-9 CAPLUS
CN Butanoic acid, 3-[[(3R)-3-[[(3S)-3-amino-5-methyl-1-oxohexyl]amino]-4-

L14 ANSWER 243 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB The clandestine synthesis of ring and side chain modified
phenylisopropylamines continues to be a major source of these drugs of
abuse. One method used for the synthesis of the amphetamine and related
compds. involves the treatment of the appropriate ketone with formamide
or
ammonium formate followed by acid hydrolysis of intermediate N-formyl
derivative In this paper the synthesis of 4-methoxyamphetamine (I, PMA)
by
the Leuckart method is investigated. The identification by means of gas
chromatog.-mass spectrometry (GC-MS) of methoxy derivative of
N-(β-phenylisopropyl)benzaldimine, methoxy derivative of
N-(β-phenylisopropyl)benzyl Me ketimine, 1-(4-methoxyphenyl)-N-(4-
methoxybenzyl)-2-propanamine, (RR/SS) and (RS)
1-(4-methoxyphenyl)-N-[2-(4-
methoxyphenyl)-1-methylethyl]-2-propanamine, (RR/SS) and

(RS)-1-(4-methoxyphenyl)-N-methyl-N-[2-(4-methoxyphenyl)-1-methylethyl]-2-
propanamine, (RR/SS) and (RS)-1-(4-methoxyphenyl)-N-formyl-N-[2-(4-
methoxyphenyl)-1-methylethyl]-2-propanamine in crude PMA, are reported.
The identity of these compds. was confirmed by independent synthesis of
reference compds. The NMR, MS, IR data, stereochem. and some chromatog.
properties of synthesized compds. are discussed. Finally, the results of
the GC-MS anal. of illicitly prepared tablets, containing PMA I and
4-methoxymethamphetamine (II, PMMA), are outlined. The presence of
4-methoxydimethylamphetamine (III), 4-methoxyethylamphetamine(IV), and
4-hydroxymethamphetamine are reported in these tablets. The identity of
II, III, and IV was confirmed by their independent synthesis.
ACCESSION NUMBER: 2002:498850 CAPLUS
DOCUMENT NUMBER: 138:132317
TITLE: Identification and synthesis of some contaminants present in 4-methoxyamphetamine (PMA) prepared by the Leuckart method
AUTHOR(S): Blachut, Dariusz; Wojtasiewicz, Krystyna; Czarnocki, Zbigniew
CORPORATE SOURCE: Department of Criminalistics, Office of the State Protection, Warsaw, 02-134, Pol.
SOURCE: Forensic Science International (2002), 127(1-2), 45-62
CODEN: FSINDR; ISSN: 0379-0738
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **475994-71-9P 475994-72-0P**
RL: BYP (Byproduct); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(identification and synthesis of some contaminants present in methoxyamphetamine prepared by Leuckart method)
RN 475994-71-9 CAPLUS
CN Benzeneethanamine, 4-methoxy-N-[(1R)-2-(4-methoxyphenyl)-1-methylethyl]-α-methyl-, (αS)-rel- (9CI) (CA INDEX NAME)

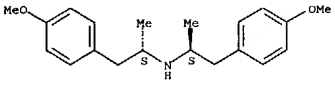
Relative stereochemistry.

L14 ANSWER 243 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 475994-72-0 CAPLUS
CN Benzeneethanamine, 4-methoxy-N-[(1R)-2-(4-methoxyphenyl)-1-methylethyl]-α-methyl-, (αR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

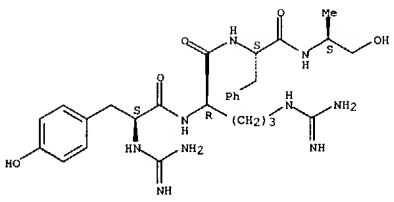
L14 ANSWER 244 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB In investigating the development of compds. with potent analgesic effects after oral administration, 74 C-terminal analogs (Nα-amidino-Tyr-D-Arg-Phe-X), based on the structure of Nα-amidino-Tyr-D-Arg-Phe-MeβAla-OH (ADAMB), were synthesized. Their analgesic activity was evaluated using the mouse-tail pressure test after both s.c. and oral administration, and the structure-activity relationships (SAR) were examined in detail. The results clearly indicated that compds. containing β-amino acid without a side chain at the X position are preferable for expression of potent analgesic activity, and that the free carboxyl group is superior in its analgesic activity to that of the esterified or amidated carboxy group at the C-terminal. In addition, N-methylation of the amide bond at the 4th position contributed to improved analgesic activity. These results indicated that the strong and long-lasting analgesic effect of ADAMB is expressed by the synergistic effects of Nα-amidination, the N-methylation of the amide bond at the 4th position and the carbon chain length (β-Ala) of the residue at the 4th position, and that this is the most suitable structure.
ACCESSION NUMBER: 2002:497653 CAPLUS
DOCUMENT NUMBER: 138:49390
TITLE: Structure-activity relationships (SAR) of [D-Arg2]dermorphin(1-4) analogues, Nα-amidino-Tyr-D-Arg-Phe-X
AUTHOR(S): Ogawa, Tadashi; Miyamae, Tetsuhisa; Okayama, Toru; Hagiwara, Masaki; Sakurada, Shinobu; Morikawa, Tadanori
CORPORATE SOURCE: Research Institute, Daiichi Fine Chemical Co., Ltd., Toyama, 933-8511, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(6), 771-780
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:49390
IT **479210-69-0P 479210-71-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure-activity relationships of dermorphin analogs)
RN 479210-69-0 CAPLUS
CN L-Phenylalaninamide, N-(aminoiminomethyl)-L-tyrosyl-D-arginyl-N-[(1S)-2-hydroxy-1-methylethyl]-, diacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 479205-52-2
CMF C28 H41 N9 O5

Absolute stereochemistry.

L14 ANSWER 244 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



CM 2

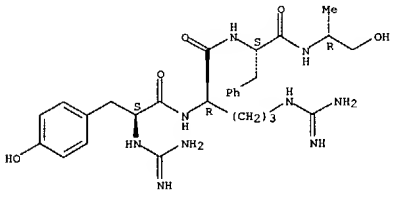
CRN 64-19-7
CMF C2 H4 O2

RN 479210-71-4 CAPLUS
CN L-Phenylalaninamide, N-(aminoiminomethyl)-L-tyrosyl-D-arginyl-N-[(1R)-2-hydroxy-1-methylethyl]-, diacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 479205-54-4
CMF C28 H41 N9 O5

Absolute stereochemistry.



CM 2

L14 ANSWER 244 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CRN 64-19-7
CMF C2 H4 O2

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 245 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI

I

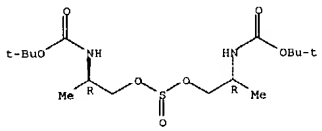
AB BOC- and dibenzosuberyl-protected chiral and hindered cyclic sulfamidates ([1,2,3]oxathiazolidine 2,2-dioxides, e.g., I) were synthesized and subsequently deprotected using trifluoroacetic acid. The resulting crystalline
sulfamidates were then used in several alkylation reactions involving benzyl bromide and alcs. in a versatile route to cyclic sulfamidates with differing N-alkyl substituents.

ACCESSION NUMBER: 2002:488378 CAPLUS
DOCUMENT NUMBER: 137:201271
TITLE: New Routes to N-Alkylated Cyclic Sulfamidates
AUTHOR(S): Posakony, Jeffrey J.; Grierson, John R.; Tewson, Timothy J.
CORPORATE SOURCE: PET Imaging Center, Department of Radiology, University of Iowa, Iowa City, IA, 52242-1007, USA
SOURCE: Journal of Organic Chemistry (2002), 67(15), 5164-5169
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:201271

IT **454248-43-2P**
RL: BYP (Byproduct); PREP (Preparation)
(new routes to N-alkylated cyclic sulfamidates)

RN 454248-43-2 CAPLUS
CN 5,7-Dioxa-6-thia-2,10-diazaundecanedioic acid, 3,9-dimethyl-, bis(1,1-dimethylethyl) ester, 6-oxide, (3R,9R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 246 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB The synthesis and separation of both diastereoisomers of 1-(4-methoxyphenyl)-N-[2-(4-methoxyphenyl)-1-methylethyl]-2-propanamine as markers of clandestine p-methoxyamphetamine were described. The stereochem. of the meso diastereomer was established by crystallog. method [monoclinic, P21/n, a 7.315(5), b 30.19(2), c 8.817(8)Å, β 95.73(7)°, V 1937(3) Å3, Z 4].

ACCESSION NUMBER: 2002:487061 CAPLUS
DOCUMENT NUMBER: 137:384595
TITLE: (2S)-1-(4-Methoxyphenyl)-N-[(1R)-2-(4-methoxyphenyl)-1-methylethyl]-2-propanamine in crude p-methoxyamphetamine (PMA) produced by the Leuckart method
AUTHOR(S): Blachut, Dariusz; Maurin, Jan K.; Starosta, Wojciech; Wojtasiewicz, Krystyna; Czarnocki, Zbigniew
CORPORATE SOURCE: Department of Criminalistics, Office of the State Protection, Warsaw, 02-134, Pol.
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (2002), 57(5), 593-597
CODEN: ZNBSEN; ISSN: 0932-0776
PUBLISHER: Verlag der Zeitschrift fuer Naturforschung
DOCUMENT TYPE: Journal
LANGUAGE: German

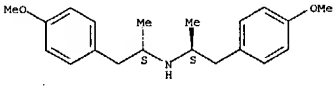
IT **475994-74-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation from 1-(4-Methoxyphenyl)-N-[2-(4-methoxyphenyl)-1-methylethyl]-2-propanamine obtained from p-methoxyamphetamine and p-methoxyphenylacetone by Leuckart method)

RN 475994-74-2 CAPLUS
CN Benzeneethanamine, 4-methoxy-N-[(1R)-2-(4-methoxyphenyl)-1-methylethyl]-α-methyl-, (αR)-rel-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 475994-72-0
CMF C20 H27 N O2

Relative stereochemistry.



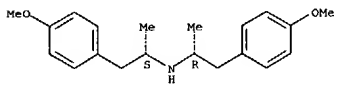
CM 2

CRN 7664-93-9
CMF H2 O4 S

IT **475994-71-9P 475994-72-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation from p-methoxyamphetamine and p-methoxyphenylacetone by Leuckart method)

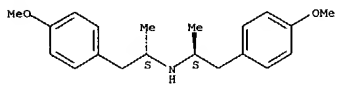
RN 475994-71-9 CAPLUS
CN Benzeneethanamine, 4-methoxy-N-[(1R)-2-(4-methoxyphenyl)-1-methylethyl]-α-methyl-, (αS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 475994-72-0 CAPLUS
CN Benzeneethanamine, 4-methoxy-N-[(1R)-2-(4-methoxyphenyl)-1-methylethyl]-α-methyl-, (αR)-rel- (9CI) (CA INDEX NAME)

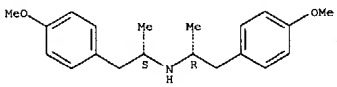
Relative stereochemistry.



IT **475994-73-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation from p-methoxyamphetamine and p-methoxyphenylacetone by Leuckart method and crystal structure)

RN 475994-73-1 CAPLUS
CN Benzeneethanamine, 4-methoxy-N-[(1R)-2-(4-methoxyphenyl)-1-methylethyl]-α-methyl-, hydrochloride, (αS)-rel- (9CI) (CA INDEX NAME)

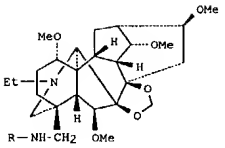
Relative stereochemistry.



● HCl

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 247 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI



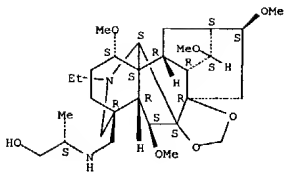
I

AB Reduction of elatidal oxime and imines based on methylamine, ethanolamine,
tyramine, and S- and (±)-alaninols gave rise to the 18-amino-18-deoxy derivs. of elatidine, I [R = H, CH2CH2OH, (S)-CHMeCH2OH, etc.].

ACCESSION NUMBER: 2002:483906 CAPLUS
DOCUMENT NUMBER: 137:279347
TITLE: Study of alkaloids of the Siberian and Altai flora. 7.
Synthesis of 18-amino-18-deoxy derivatives of elatidine
AUTHOR(S): Ganbaatar, J.; Batsuren, D.; Osadchii, S. A.; Shults, E. E.; Tolstikov, G. A.
CORPORATE SOURCE: Institute of Chemistry and Chemical Technology, Mongolian Academy of Sciences, Ulan-Bator, 211051, Mongolia
SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (2002), 51(3), 531-534
CODEN: RCBUEY; ISSN: 1066-5285
PUBLISHER: Kluwer Academic/Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **464881-02-5P 464881-05-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of aminodeoxy derivs. of elatidine via reduction of elatidal oxime
and imines)
RN 464881-02-5 CAPLUS
CN 1-Propanol, 2-[[[(1α,6β,14α,16β)-20-ethyl-1,6,14,16-tetramethoxy-7,8-[methylenebis(oxy)]aconitan-4-yl]methyl]amino]-, (2S)-(9CI) (CA INDEX NAME)

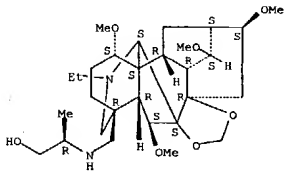
Absolute stereochemistry. Rotation (+).

L14 ANSWER 247 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 464881-05-8 CAPLUS
CN 1-Propanol, 2-[[[(1α,6β,14α,16β)-20-ethyl-1,6,14,16-tetramethoxy-7,8-[methylenebis(oxy)]aconitan-4-yl]methyl]amino]-, (2R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



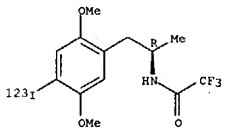
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 248 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB Our goal was to synthesize with high specific activity R(-)-1-(2,5-Dimethoxy-4-[123I]iodophenyl)-2-aminopropane [R(-)[123I]DOI], an in vitro potent and selective 5-HT2A/2C serotonin agonist, and study in
vivo its plasma pharmacokinetics and brain distribution in baboon by SPECT. The purpose was to evaluate this radiotracer as a potential tool in discerning the role of the agonist high affinity state of 5-HT2 receptors in depression and other neurol. disorders.The radiotracer was prepared by electrophilic radioiodination of the N-trifluoroacetyl precursor
of R(-)-1-(2,5-Dimethoxyphenyl)-2-aminopropane [R(-)DMA-TFA] with high-purity sodium [123I]iodide in the presence of chloramine-T, followed by amino deprotection with KOH in isopropanol (labeling yield: 73%, radiochem. yield: 62%, radiochem. purity: 99%). In vivo studies in baboon
showed high accumulation of radioactivity in thalamus, the frontoparietal cortex, temporal, occipital and the striatum regions, with slightly lower accumulation in the midbrain and cerebellum. Ketanserin did not displaced
the radioactivity in any of these brain regions.Plasma metabolite anal. was performed using methanol protein precipitation, the methanol fractions
contained from 68% to 92% of the mixture of a labeled metabolite and parent
compound The recovery coefficient of unmetabolized R(-)[123I]DOI was 68%. The
percent parent compound present in the extracted fraction, measured by HPLC,
decreased gradually with time from 99.8% to 0.3% still present after 4.7 h
post injection whereas the percentage of the only one detected metabolite increased conversely. Free fraction determination (f1), was 31 ± 0.9% (n = 3).
For comparison purposes, ex-vivo brain distribution, displacement and metabolite anal. was also carried out in rodents.Although R(-)[123I]DOI displayed good brain uptake and localized in serotonergic areas of the brain, its target to non target ratio and its insensitivity to ketanserin displacement suggest high nonspecific uptake, therefore non potentially useful as brain imaging radiotracer for visualization of the agonist high-affinity state of 5-HT2A receptors and for visualizing 5-HT2C receptors by SPECT.

ACCESSION NUMBER: 2002:476219 CAPLUS
DOCUMENT NUMBER: 138:165760
TITLE: Pharmacokinetics and brain distribution in non human primate of R(-)[123I]DOI, A 5HT2A/2C serotonin agonist
AUTHOR(S): Zea-Ponce, Yolanda; Kegeles, Lawrence S.; Guo, Ningning; Raskin, Leonid; Bakthavachalam, Venkatesalu;
Laruelle, Marc
CORPORATE SOURCE: Departments of Psychiatry and Radiology, Columbia University College of Physicians and Surgeons, New York, NY, USA
SOURCE: Nuclear Medicine and Biology (2002), 29(5), 575-583
CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **497182-37-3P**

L14 ANSWER 248 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(pharmacokinetics and brain distribution of R(-)[123]DOI, A 5HT2A/2C serotonin agonist)
RN 497182-37-3 CAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1R)-2-[4-(iodo-123I)-2,5-dimethoxyphenyl]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 249 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

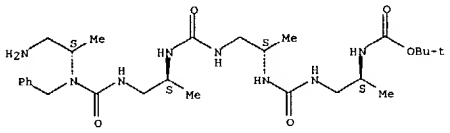
AB Square-shaped hydrogen-bonded polar nanotubes are formed when the C4-sym. all-S cyclotetraurea bearing side chains of alanine self-assembles in the solid state. The four urea fragments in the macrocycle present an all-trans planar conformation with an unidirectional alignment of all the carbonyl groups. The anisotropy is further maintained in the crystal as neighboring tubes are all arranged in the same direction.

ACCESSION NUMBER: 2002:471573 CAPLUS
DOCUMENT NUMBER: 137:294567
TITLE: Self-assembling organic nanotubes from enantiopure cyclo-N,N'-linked oligoureas: Design, synthesis, and crystal structure
AUTHOR(S): Semetey, Vincent; Didierjean, Claude; Briand, Jean-Paul; Aubry, Andre; Guichard, Gilles
CORPORATE SOURCE: Immunologie et Chimie Therapeutiques, UPR CNRS 9021 Institut de Biologie Moleculaire et Cellulaire, Strasbourg, 67084, Fr.
SOURCE: Angewandte Chemie, International Edition (2002), 41(11), 1895-1898
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **467424-41-5P 467424-48-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and crystallog. of self-assembling organic nanotubes from enantiopure cyclo-N,N'-linked oligoureas)

RN 467424-41-5 CAPLUS
CN 2,5,7,10,12,15,17-Heptaazanonadecanoic acid, 19-amino-3,8,13,18-tetramethyl-6,11,16-trioxo-17-(phenylmethyl)-, 1,1-dimethylethyl ester, conjugate monoacid, (3S,8S,13S,18S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

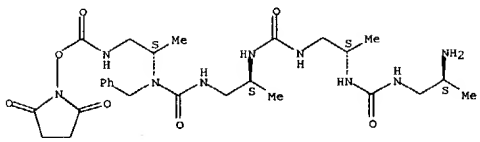


● H^+

RN 467424-48-2 CAPLUS
CN 2,5,7,10-Tetraazaundecanediamide, N1-[(2S)-2-aminopropyl]-N11-[(1S)-2-[[[(2,5-dioxo-1-pyrrolidinyl)oxy]carbonyl]amino]-1-methylethyl]-3,8-dimethyl-6-oxo-N11-(phenylmethyl)-, conjugate monoacid, (3S,8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

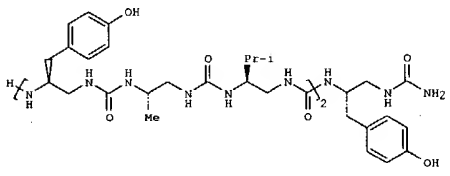
L14 ANSWER 249 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



● H^+

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 250 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I

AB The solution structure of heptaurea I bearing side chains of natural amino acids Ala, Val, and Tyr is reported. Oligourea I was prepared by solid-phase synthesis and its structure was investigated by 1D and 2D NMR spectroscopy. The spin systems of all seven residues were identified from DQF-COSY and TOCSY expts., the sequence and three-dimensional structure of I were assigned on the basis of ROESY expts. Chemical shifts and coupling consts. for backbone protons of residue 3 strongly suggested that oligourea I adopts in solns. a well-defined right-handed 2.5 helical secondary structure with the simultaneous presence of 12- and 14-membered hydrogen-bonded rings.

ACCESSION NUMBER: 2002:471572 CAPLUS
DOCUMENT NUMBER: 137:217233
TITLE: Stable helical secondary structure in short-chain N,N'-linked oligoureas bearing proteinogenic side chains
AUTHOR(S): Semetey, Vincent; Rognan, Didier; Hemmerlin, Christine; Graff, Roland; Briand, Jean-Paul; Marraud, Michel; Guichard, Gilles
CORPORATE SOURCE: Immunologie et Chimie Therapeutiques, UPR CNRS 9021 Institut de Biologie Moleculaire et Cellulaire, Strasbourg, 67084, Fr.
SOURCE: Angewandte Chemie, International Edition (2002), 41(11), 1893-1895
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:217233

IT **455323-81-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis and three-dimensional helical secondary structure of heptaurea in solns.)

RN 455323-81-6 CAPLUS
CN 2,5,7,10,12,15,17,20,22,25,27,30-Dodecaazahentriacontanediamide, N1-[(2S)-2-amino-3-(4-hydroxyphenyl)propyl]-13,28-bis[(4-

L14 ANSWER 250 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

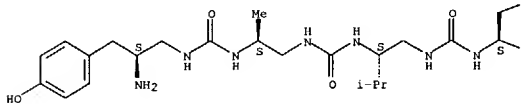
hydroxyphenyl)methyl]-3,18-dimethyl-8,23-bis(1-methylethyl)-6,11,16,21,26-pentaoxo-, (3S,8S,13S,18S,23S,28S)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

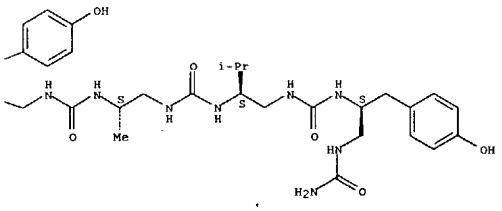
CRN 270575-79-6
CMF C50 H79 N15 O10

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CM 2

CRN 76-05-1
CMF C2 H F3 O2

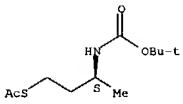
L14 ANSWER 250 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 251 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB Fibroblast collagenase (MMP-1), a member of the matrix metalloproteinases family, is believed to be a pathogenesis of arthritis, by cleaving triple-helical type II collagen in cartilage. From the similarity of the active site zinc binding mode with hydroxamate, we designed and synthesized α-mercaptocarbonyl possessing compds. which incorporated various peptide sequences as enzyme recognition sites. The P4-P1 peptide incorporating compound (S)-Ph-C(O)-Gly-Pro-Leu-NHCH(CH3)C(O)CH2SH (I) exhibited as potent inhibition as the hydroxamate and the carboxylate type
inhibitors, with an IC50 of 10-6 M order against MMP-1. But the inhibitor
I related compds. in which terminal C(O)CH2SH was replaced by (CH2)2SH, C(O)(CH2)2SH, or CH(OH)CH2SH, displayed decreased or no inhibitory potencies. These results suggest that the existence of both the carbonyl and thiol groups might be critical for the inhibition, and the distance between the two functional groups is important for inhibitory potency. Several Pn' peptide incorporating compds. showed IC50 values under sub-nanomolar. Among them, for potent inhibition, Leu was better than Phe
and Val as the P1' amino acid, and the P2' position amino acid was necessary, and preferentially Phe. Substitution of the mercapto group with other functional groups lost the activity of unsubstituted compound The stereochem. preference at the thiol-attached position was also determined
It was found that the S configuration compound is approx. 100 times more potent than the corresponding R-isomer.
ACCESSION NUMBER: 2002:469786 CAPLUS
DOCUMENT NUMBER: 137:232899
TITLE: Design and synthesis of sulfur based inhibitors of matrix metalloproteinase-1
AUTHOR(S): Fujisawa, Tetsunori; Odake, Shinjiro; Ogawa, Yuji; Yasuda, Junko; Morita, Yasuo; Morikawa, Tadanori
CORPORATE SOURCE: Research Institute, Fuji Chemical Industries, Ltd., Toyama, 933-8511, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(2), 239-252
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:232899
IT **458531-55-0P 458531-63-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of in the preparation of peptide-mercapto compds.)
RN 458531-55-0 CAPLUS
CN Ethanethioic acid, S-[(3S)-3-[[(1,1-dimethylethoxy)carbonyl]amino]butyl] ester (9CI) (CA INDEX NAME)

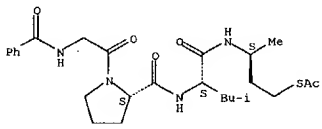
Absolute stereochemistry. Rotation (-).

L14 ANSWER 251 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 458531-63-0 CAPLUS
CN L-Leucinamide, N-benzoylglycyl-L-prolyl-N-[(1S)-3-(acetylthio)-1-methylpropyl]- (9CI) (CA INDEX NAME)

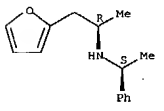
Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

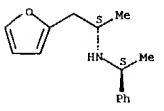
L14 ANSWER 252 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB The preparation of enantiomerically pure δ- and γ-sultams by intramol. [4+2] cycloaddn. of N-1-phenylethyl substituted vinylsulfonamides with purely thermal activation and under high pressure was discussed. An optimized procedure for reductive debenzylation of the resultant δ-sultams is also reported.
ACCESSION NUMBER: 2002:456635 CAPLUS
DOCUMENT NUMBER: 138:24684
TITLE: Preparation of enantiopure sultams by intramolecular Diels-Alder reaction of furan-containing vinylsulfonamides
AUTHOR(S): Rogatchov, Viktor O.; Bernsmann, Heiko; Schwab, Pia; Frohlich, Roland; Wibbeling, Birgit; Metz, Peter
CORPORATE SOURCE: Institut fur Organische Chemie, Technische Universitat
Dresden, Dresden, D-01069, Germany
SOURCE: Tetrahedron Letters (2002), 43(27), 4753-4756
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:24684
IT **477788-38-8 477788-40-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of racemic furan derivs. as starting materials in synthesis of
enantiopure sultams)
RN 477788-38-8 CAPLUS
CN 2-Furanethanamine, α-methyl-N-[(1S)-1-phenylethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 477788-40-2 CAPLUS
CN 2-Furanethanamine, α-methyl-N-[(1S)-1-phenylethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 252 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L14 ANSWER 253 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

AB The structural properties of an all-β3-dodecapeptide with the sequence H-β-HLys(N.vepsiln.-CO(CH2)3-S-Acm)-β-HPhe-β-HTyr-β-HLeu-β-HLys-β-HSer-β-HLys-β-HPhe-β-HSer-β-HVal-β-HLys-β-HAla-OH (1) have been studied by two-dimensional homonuclear 1H-NMR and by CD spectroscopy. In MeOH solution, high-resolution NMR spectroscopy showed that the β-dodecapeptide forms an (M)-314-helix, and the CD spectrum corresponds to the pattern expected for an (M)-314-helical secondary structure. In aqueous solution, however, the peptide adopts a predominantly extended conformation without regular secondary-structure elements, which is in agreement with the absence of the characteristic trough near 215 nm in the CD spectrum. The NMR and CD measurements with solns. of 1 in MeOH containing 3M urea further indicated that the peptide retains the regular secondary structural elements under these conditions, whereas, after addition of 40% (volume/volume) H2O to the MeOH solution, the large 1H-chemical-shift dispersion indicative of a defined spatial peptide fold was lost. The β3-dodecapeptide is - so far - the longest β-peptide shown to adopt a regular (M)-314-helix conformation in an organic solvent. The observation that the structure of this long β3-peptide is not maintained in aqueous solution indicates that the (M)-314-fold is primarily stabilized by short-range interactions.

ACCESSION NUMBER: 2002:451992 CAPLUS
DOCUMENT NUMBER: 137:201596
TITLE: NMR-structural investigations of a β3-dodecapeptide with proteinogenic side chains in methanol and in aqueous solutions
AUTHOR(S): Etezady-Esfarjani, Touraj; Hilty, Christian; Wuethrich, Kurt; Rueping, Magnus; Schreiber, Juerg; Seebach, Dieter
CORPORATE SOURCE: Institut fuer Molekularbiologie und Biophysik, Eidgenoessischen Technischen Hochschule Zurich, Zurich, CH-8093, Switz.
SOURCE: Helvetica Chimica Acta (2002), 85(5), 1197-1209
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English

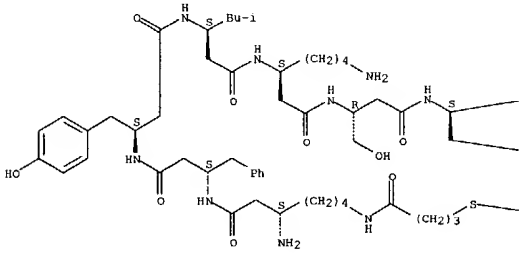
IT **454486-18-1P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(secondary and tertiary structure of prepared on solid phase β3-dodecapeptide in methanol and in aqueous solns. by NMR, CD and statistical calcn.)

RN 454486-18-1 CAPLUS
CN 5-Thia-3,10,18,22,26,30,34,38,42,46,50,54,58-tridecaazahenhexacontan-61-oic acid, 15-amino-31,39,55-tris(4-aminobutyl)-35,47-bis(hydroxymethyl)-23-[(4-hydroxyphenyl)methyl]-59-methyl-51-(1-methylethyl)-27-(2-methylpropyl)-2,9,17,21,25,29,33,37,41,45,49,53,57-tridecaoxo-19,43-bis(phenylmethyl)-, (15S,19S,23S,27S,31S,35R,39S,43S,47R,51R,55S,59S)- (9CI) (CA INDEX NAME)

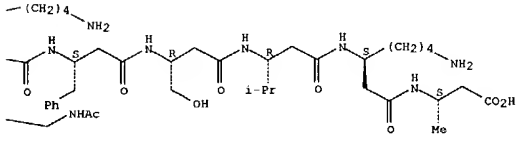
L14 ANSWER 253 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 55 THIS FORMAT
THERE ARE 55 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

L14 ANSWER 254 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

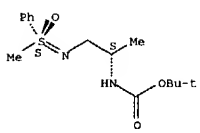
AB N-Alkylated sulfoximines have been synthesized in good yields by acylation of NH-sulfoximines followed by carbonyl reduction with complexed boranes. Enantiopure substrates react without racemization and stereogenic centers originating from the acylating component are retained. If the acylation is performed by DCC coupling, this two-step procedure represents a rare example of a formal N-alkylation of sulfoximines under base-free conditions.

ACCESSION NUMBER: 2002:414663 CAPLUS
DOCUMENT NUMBER: 137:325201
TITLE: A mild synthetic procedure for the preparation of N-alkylated sulfoximines
AUTHOR(S): Bolm, Carsten; Hackenberger, Christian P. R.; Simic, Oliver; Verrucci, Marinella; Muller, Dirk; Bienewald, Frank
CORPORATE SOURCE: Institut fur Organische Chemie der RWTH Aachen, Aachen, 52056, Germany
SOURCE: Synthesis (2002), (7), 879-887
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **473441-43-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(mild procedure for the preparation of N-alkylated sulfoximines)

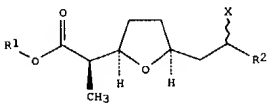
RN 473441-43-9 CAPLUS
CN Sulfoximine, N-[(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]-S-methyl-S-phenyl-, [S(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

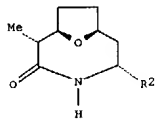


REFERENCE COUNT: 66 THIS FORMAT
THERE ARE 66 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

L14 ANSWER 255 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I



II

AB Novel THF-amino acids were efficiently synthesized from actic acid Me esters. The conformational restriction imposed by the 2,5-cis disubstituted THF moiety is apparent from their facile cyclization to give medium-sized lactams. Thus, treatment of actic acid Me ester [I; wherein R1 = Me; X = OH; R2 = Me] with triphenylphosphine dibromide gives [I; wherein R1 = Me; X = Br; R2 = Me], which is reacted with sodium azide to give [I; wherein R1 = Me; X = N3; R2 = Me], and after hydrogenation and saponification, [II; wherein R2 = Me] is formed.

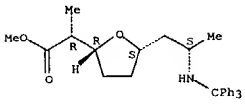
ACCESSION NUMBER: 2002:379146 CAPLUS
DOCUMENT NUMBER: 137:294828
TITLE: Amino analogs of actic acids-synthesis and lactamization
AUTHOR(S): Bernsmann, Heiko; Wang, Yuzhou; Frohlich, Roland; Metz, Peter
CORPORATE SOURCE: Institut fur Organische Chemie, Technische Universitat
Dresden, Dresden, D-01069, Germany
SOURCE: Tetrahedron (2002), 58(22), 4451-4457
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:294828

IT **468057-36-5P 468057-37-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino analogs of actic acids and their lactamization)

RN 468057-36-5 CAPLUS
CN 2-Furanacetic acid, tetrahydro-α-methyl-5-[(2S)-2-[(triphenylmethyl)amino]propyl]-, methyl ester, (αR,2R,5S)- (9CI)

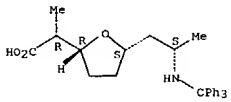
L14 ANSWER 255 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



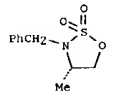
RN 468057-37-6 CAPLUS
CN 2-Furanacetic acid, tetrahydro-α-methyl-5-[(2S)-2-[(triphenylmethyl)amino]propyl]-, (αR,2R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



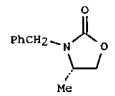
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 256 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
GI

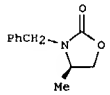


I

II



III



IV

AB N-benzyl [1,2,3]-oxathiazolidine 2,2-dioxides, e.g. I, (cyclic sulfamidates) were synthesized from their corresponding β-amino alcs. and used as substrates in fluorination reactions with tetrabutylammonium fluoride (TBAF). After desulfonation of the intermediates, the N-benzyl fluoroamines were debenzylated by transfer hydrogenolysis with Pd/C to yield (S) and (R)-2-amino-1-fluoropropane hydrochloride salts (II, both with 95% ee). The reactions were carried out on multi-gram scale without the need for chromatog. purification of the intermediates. In the presence of carbonate, the (S)- and (R)-N-benzylfluoroamines underwent intramol. cyclizations in which fluoride was displaced to yield cyclic carbamates III and IV.

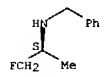
ACCESSION NUMBER: 2002:370219 CAPLUS
DOCUMENT NUMBER: 137:232363
TITLE: Fluoroamines via chiral cyclic sulfamidates
AUTHOR(S): Posakony, Jeffrey J.; Tewson, Timothy J.
CORPORATE SOURCE: Department of Radiology Imaging Research Laboratory, University of Washington, Seattle, WA, 98195, USA
SOURCE: Synthesis (2002), (6), 766-770
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:232363

IT **458560-73-1P 458560-75-3P 458560-83-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluoroamines via chiral cyclic sulfamidates)

RN 458560-73-1 CAPLUS
CN Benzenemethanamine, N-[(1S)-2-fluoro-1-methylethyl]- (9CI) (CA INDEX NAME)

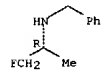
Absolute stereochemistry. Rotation (+).

L14 ANSWER 256 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



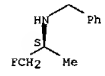
RN 458560-75-3 CAPLUS
CN Benzenemethanamine, N-[(1R)-2-fluoro-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 458560-83-3 CAPLUS
CN Benzenemethanamine, N-[(1S)-2-fluoro-1-methylethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

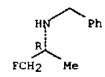


● HCl

IT **458560-86-6P 458560-91-3P 458560-94-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(fluoroamines via chiral cyclic sulfamidates)

RN 458560-86-6 CAPLUS
CN Benzenemethanamine, N-[(1R)-2-fluoro-1-methylethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

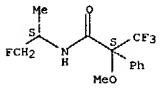


● HCl

RN 458560-91-3 CAPLUS

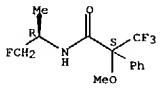
L14 ANSWER 256 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN Benzeneacetamide, N-[(1S)-2-fluoro-1-methylethyl]-α-methoxy-α-(trifluoromethyl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 458560-94-6 CAPLUS
CN Benzeneacetamide, N-[(1R)-2-fluoro-1-methylethyl]-α-methoxy-α-(trifluoromethyl)-, (αS)- (9CI) (CA INDEX NAME)

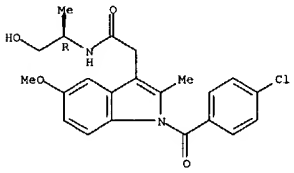
Absolute stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 257 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN
AB Cyclooxygenase inhibition studies with novel indomethacin alkanolamides demonstrate the potential for dramatic differences in inhibitor properties conferred by subtle structural modifications. The transformation of non-selective α-(S)-substituted indomethacin ethanolamides to potent, COX-2 selective inhibitors by simple stereocenter inversion highlights this property.
ACCESSION NUMBER: 2002:287803 CAPLUS
DOCUMENT NUMBER: 137:362491
TITLE: Enantiospecific, selective cyclooxygenase-2 inhibitors
AUTHOR(S): Kozak, Kevin R.; Prusakiewicz, Jeffery J.; Rowlinson, Scott W.; Marnett, Lawrence J.
CORPORATE SOURCE: Departments of Biochemistry and Chemistry, Vanderbilt University School of Medicine, Vanderbilt-Ingram Cancer Center and Center in Molecular Toxicology, Nashville, TN, 37232, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(9), 1315-1318
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **475589-54-9 475589-55-0 475589-73-2 475589-74-3 475589-75-4 475589-76-5**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(structure-activity relationship studies of enantiospecific, selective cyclooxygenase-2 inhibitors)
RN 475589-54-9 CAPLUS
CN 1H-Indole-3-acetamide, 1-(4-chlorobenzoyl)-N-[(1R)-2-hydroxy-1-methylethyl]-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)

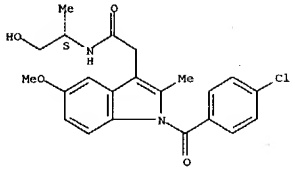
Absolute stereochemistry.



RN 475589-55-0 CAPLUS
CN 1H-Indole-3-acetamide, 1-(4-chlorobenzoyl)-N-[(1S)-2-hydroxy-1-methylethyl]-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)

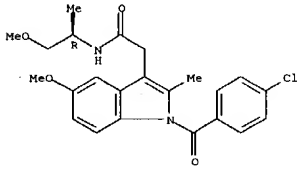
Absolute stereochemistry.

L14 ANSWER 257 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



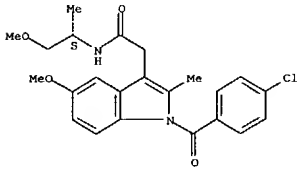
RN 475589-73-2 CAPLUS
CN 1H-Indole-3-acetamide, 1-(4-chlorobenzoyl)-5-methoxy-N-[(1R)-2-methoxy-1-methylethyl]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



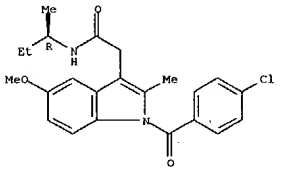
RN 475589-74-3 CAPLUS
CN 1H-Indole-3-acetamide, 1-(4-chlorobenzoyl)-5-methoxy-N-[(1S)-2-methoxy-1-methylethyl]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



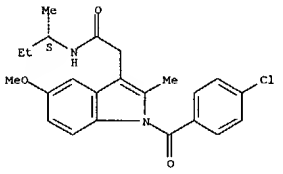
RN 475589-75-4 CAPLUS
CN 1H-Indole-3-acetamide, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-N-[(1R)-1-methylpropyl]- (9CI) (CA INDEX NAME)

L14 ANSWER 257 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Absolute stereochemistry.



RN 475589-76-5 CAPLUS
CN 1H-Indole-3-acetamide, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-N-[(1S)-1-methylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 258 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

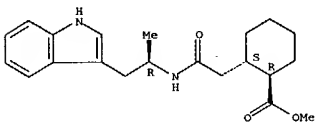
AB Some time ago, Siddiqui et al. proposed a structure for the naturally occurring indole alkaloid yohambinine, which had been isolated from Rauwolfia serpentina BENTH. In the present paper, enantioselective syntheses of all eight diastereoisomers endowed with the proposed 5-methylyohimbane structure are disclosed. However, none of the synthetically prepared compds. showed spectroscopic properties identical to those reported for the natural product yohambinine, which, therefore, must possess an altogether different constitutional formula. The ground-state conformations of the diastereoisomers were deduced by spectroscopic methods, and the outcome was compared with the results of extensive force-field, semi-empirical, and ab-initio calcns.

ACCESSION NUMBER: 2002:284207 CAPLUS
DOCUMENT NUMBER: 137:185691
TITLE: Synthesis and conformational analysis of all eight diastereoisomers of 5-methylyohimbane
AUTHOR(S): Lohse, Christian; Detterbeck, Richard; Acklin, Pierre; Borschberg, Hans-Jurg
CORPORATE SOURCE: Laboratorium fur Organische Chemie der Eidgenossischen Technischen Hochschule, HCl, ETH-Honggerberg, Zurich, CH-8093, Switz.
SOURCE: Helvetica Chimica Acta (2002), 85(3), 945-961
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:185691

IT **451498-62-7P 451498-72-9P 451498-88-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and conformational anal. of 5-methylyohimbane diastereomers)

RN 451498-62-7 CAPLUS
CN Cyclohexanecarboxylic acid, 2-[2-[[(1R)-2-(1H-indol-3-yl)-1-methylethyl]amino]-2-oxoethyl]-, methyl ester, (1R,2S)- (9CI) (CA INDEX NAME)

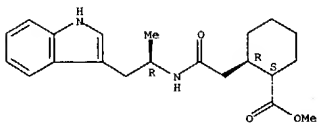
Absolute stereochemistry. Rotation (-).



RN 451498-72-9 CAPLUS
CN Cyclohexanecarboxylic acid, 2-[2-[[(1R)-2-(1H-indol-3-yl)-1-methylethyl]amino]-2-oxoethyl]-, methyl ester, (1S,2R)- (9CI) (CA INDEX NAME)

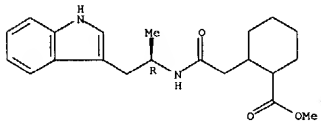
Absolute stereochemistry. Rotation (+).

L14 ANSWER 258 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 451498-88-7 CAPLUS
CN Cyclohexanecarboxylic acid, 2-[2-[[(1R)-2-(1H-indol-3-yl)-1-methylethyl]amino]-2-oxoethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 259 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

AB To determine the structural requirements for cellular uptake of β-peptides, a series of fluorescein-labeled β-peptides was prepared 3T3 mouse fibroblast cells were cultured as exponentially growing monolayers in RPMI 1640 medium, without phenol red, supplemented with 10% fetal calf serum and 1 mm glutamine at 37 under 5% CO2. The ability of fluorescence-labeled peptides to enter the cells was analyzed by fluorescence microscopy. Results demonstrate the ability of polycationic β-peptides to internalize into cells. It was found that β-oligoarginine was significantly more effective in entering cells than β-oligolysine. Because of their resistance to enzyme degradation, it is possible to use β-oligoarginine derivs. for long-term binding to cell nuclei.

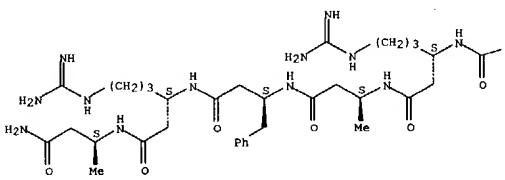
ACCESSION NUMBER: 2002:266166 CAPLUS
DOCUMENT NUMBER: 137:163274
TITLE: Cellular uptake studies with β-peptides
AUTHOR(S): Rueping, Magnus; Mahajan, Yogesh; Sauer, Markus; Seebach, Dieter
CORPORATE SOURCE: Laboratorium fur Organische Chemie der Eidgenossischen Technischen Hochschule ETH-Honggerberg, Zurich, 8093, Switz.
SOURCE: ChemBioChem (2002), 3(2-3), 257-259
CODEN: CBCHFX; ISSN: 1439-4227
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **447408-08-4 447408-09-5 447408-11-9**
RL: PKT (Pharmacokinetics); BIOL (Biological study)
(cellular uptake studies with β-peptides)

RN 447408-08-4 CAPLUS
CN 2,6,10,14,18,22,26-Heptaazanonacosan-29-amide, 11,23-bis[3-[(aminoiminomethyl)amino]propyl]-1-[2-(6-hydroxy-3-oxo-3H-xanthen-9-yl)phenyl]-3,15,27-trimethyl-1,5,9,13,17,21,25-heptaoxo-7,19-bis(phenylmethyl)-, (3S,7S,11S,15S,19S,23S,27S)- (9CI) (CA INDEX NAME)

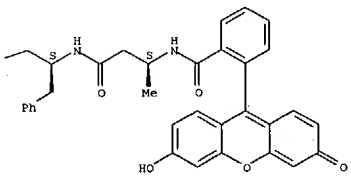
Absolute stereochemistry.

PAGE 1-A



L14 ANSWER 259 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

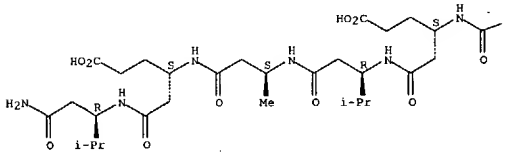
PAGE 1-B



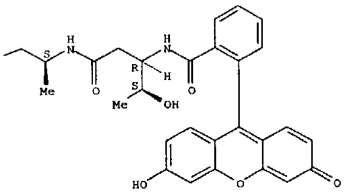
RN 447408-09-5 CAPLUS
CN 2,6,10,14,18,22-Hexaazahexacosan-26-oic acid, 23-[2-[[(1R)-3-amino-1-(1-methylethyl)-3-oxopropyl]amino]-2-oxoethyl]-11-(2-carboxyethyl)-3-[(1S)-1-hydroxyethyl]-1-[2-(6-hydroxy-3-oxo-3H-xanthen-9-yl)phenyl]-7,19-dimethyl-15-(1-methylethyl)-1,5,9,13,17,21-hexaoxo-, (3R,7S,11S,15R,19S,23S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



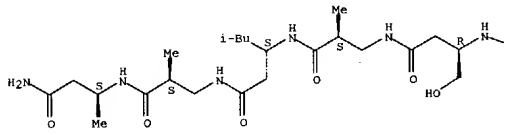
PAGE 1-B



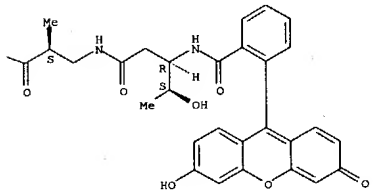
RN 447408-11-9 CAPLUS
CN 2,6,10,14,18,22,26-Heptaazanonacosan-29-amide,
3-[(1S)-1-hydroxyethyl]-11-
(hydroxymethyl)-1-[2-(6-hydroxy-3-oxo-3H-xanthen-9-yl)phenyl]-8,16,24,27-
tetramethyl-19-(2-methylpropyl)-1,5,9,13,17,21,25-heptaoxo-,
(3R,8S,11R,16S,19S,24S,27S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
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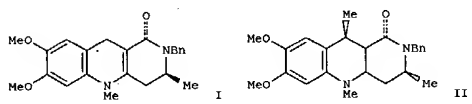
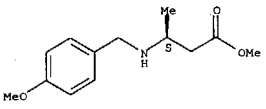


I II

AB The authors report the stereoselective synthesis of new chiral NADH mimics
I and II of the benzo[b]-1,6-naphthryridine series. The synthesis of I and II relies upon a Friedlander-type condensation between an amino imine and piperidine-2,4-dione bearing a stereogenic center at C(6). The resulting NADH models were involved in the reduction of Me benzoylformate. A
comparison of their performance with that of previously reported NADH mimics throws new light on the role played by the C(4)-C(3)-C:O dihedral angle (α) on the stereoselectivity of the hydride transfer.

ACCESSION NUMBER: 2002:252132 CAPLUS
DOCUMENT NUMBER: 137:200922
TITLE: Influence of the C(4)-C(3)-C:O dihedral angle of chiral NADH mimics on the stereoselectivity of reductions
AUTHOR(S): Vasse, Jean-Luc; Levacher, Vincent; Bourguignon, Jean;
Dupas, Georges
CORPORATE SOURCE: Laboratoire de Chimie Organique, Fine et Heterocyclique associe au CNRS, IRCOF-INSA, Mont Saint
Aignan, F-76131, Fr.
SOURCE: Tetrahedron: Asymmetry (2002), 13(3), 227-232
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:200922
IT **453556-44-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(influence of the C(4)-C(3)-C:O dihedral angle of chiral NADH mimics on
the stereoselectivity of redns.)
RN 453556-44-0 CAPLUS
CN Butanoic acid, 3-[[(4-methoxyphenyl)methyl]amino]-, methyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 261 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

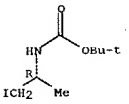
AB A concise route to enantiomerically pure 2-substituted indolines and a 2-substituted tetrahydroquinoline has been developed by application of the Pd-catalyzed coupling of amino functionalized organozinc reagents with 2-bromoiodobenzene, followed by Buchwald's palladium-catalyzed intramol. amination reaction. The yields in the initial coupling are modest (36-52%), but the cyclization yields are satisfactory (63-87%). The stereochem. integrity of a representative example was established by chiral phase HPLC.

ACCESSION NUMBER: 2002:173497 CAPLUS
DOCUMENT NUMBER: 137:169388
TITLE: Synthesis of 2-substituted indolines using sequential Pd-catalyzed processes
AUTHOR(S): Deboves, Herve J. C.; Hunter, Christopher; Jackson, Richard F. W.
CORPORATE SOURCE: Department of Chemistry, The University of Newcastle, Newcastle upon Tyne, NE1 7RU, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1
(2002), (6), 733-736
CODEN: JCSPCE; ISSN: 1472-7781
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:169388

IT **446060-78-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-substituted indolines using sequential Pd-catalyzed processes)

RN 446060-78-2 CAPLUS
CN Carbamic acid, [(1R)-2-iodo-1-methylethyl]-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

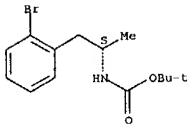


IT **446059-15-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-substituted indolines using sequential Pd-catalyzed processes)

RN 446059-15-0 CAPLUS
CN Carbamic acid, [(1S)-2-(2-bromophenyl)-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

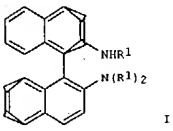
L14 ANSWER 261 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 262 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN

GI



I

AB Triacylbinaphthylamines I (R1 = (halo-substituted) alkanoyl] are prepared H2NCR2R3 (II; R2, R3 = organic group; R2 ≠ R3) are optically resolved by N-acylation of one optical isomer of II with I, isolation, and deacylation. I (R1 = H) was reacted with Ac2O in pyridine at 100° for 24 h to give 65% I (R1 = Ac). α-Methylbenzylamine was acylated with I (R1 = Ac) in DMSO at room temperature for 3 h to give 24% (S)-N-acetyl-α-methylbenzylamine with 30% e.e.

ACCESSION NUMBER: 1999:631118 CAPLUS
DOCUMENT NUMBER: 131:243085
TITLE: Preparation of optically active triacylbinaphthylamines and optical resolution of amines with them
INVENTOR(S): Murakami, Yasuoki; Kondo, Kazuhiro
PATENT ASSIGNEE(S): Shiratori Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11269133	A2	19991005	JP 1998-72103	19980320

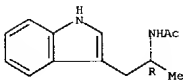
PRIORITY APPLN. INFO.: JP 1998-72103 19980320
OTHER SOURCE(S): CASREACT 131:243085; MARPAT 131:243085

IT **660846-14-0P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active triacylbinaphthylamines and optical resolution of amines by acylation with them)

RN 660846-14-0 CAPLUS
CN Acetamide, N-[(1R)-2-(1H-indol-3-yl)-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 262 OF 262 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY     SESSION
FULL ESTIMATED COST                                  302.73      495.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY     SESSION
CA SUBSCRIBER PRICE                                  -43.66      -47.82

FILE 'REGISTRY' ENTERED AT 16:54:41 ON 05 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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STRUCTURE FILE UPDATES:     4 MAY 2004  HIGHEST RN 679784-15-7
DICTIONARY FILE UPDATES:    4 MAY 2004  HIGHEST RN 679784-15-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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Uploading C:\Program Files\Stnexp\Queries\09857465.str
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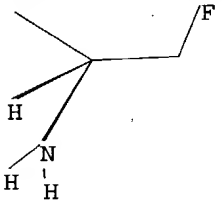

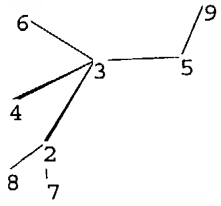


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chain nodes :
2  3  4  5  6  7  8  9
chain bonds :
2-3  2-7  2-8  3-4  3-5  3-6  5-9
exact/norm bonds :
2-3
exact bonds :
2-7  2-8  3-4  3-5  3-6  5-9


G1:H,F

Match level :
2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:CLASS  9:CLASS

Stereo Bonds:
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3-2 (Single Wedge).
4-3 (Single Hash).

Stereo Chiral Centers:

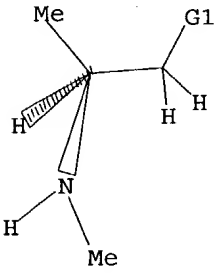
3 (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 3

L15 STRUCTURE UPLOADED

=> d query
L15 STR



G1 H,F

Structure attributes must be viewed using STN Express query preparation.

=> s l15
SAMPLE SEARCH INITIATED 16:54:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 115437 TO ITERATE

0.9% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 0

L16 0 SEA SSS SAM L15

=> s l15 exact
STRUCTURES CONTAINING VARIABLE NODES NOT VALID IN EXACT OR FAMILY SEARCH
You have requested a full structure (EXA or FAM) search on a
structure containing one of the special variable-atom symbols
A, M, Q, or X, or a variable group G. Only bond variability
is allowed in structures for EXA or FAM searches. Variable
nodes are never permitted.

=> s l15 full
FULL SEARCH INITIATED 16:55:15 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 17.3% PROCESSED 400000 ITERATIONS 47 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.13

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 222

L17 47 SEA SSS FUL L15

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	650.58

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-47.82

FILE 'CAPLUS' ENTERED AT 16:55:31 ON 05 MAY 2004
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FILE COVERS 1907 - 5 May 2004 VOL 140 ISS 19
FILE LAST UPDATED: 4 May 2004 (20040504/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l17
L18 12 L17

=> d l18 1-12 abs ibib hitstr

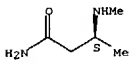
L18 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

AB Partially modified retro- (PMR) and retro-inverso (PMRI) ψ[NHCH(CF3)]Gly peptides, a conceptually new class of peptidomimetics, have been synthesized in wide structural diversity and variable length by aza-Michael reaction of enantiomerically pure α-amino esters and peptides with enantiomerically and geometrically pure N-(4,4,4-trifluorocrotonoyl)oxazolidin-2-ones. The factors underlying the observed moderate to good diastereocontrol have been investigated. The conformations of model PMR-ψ[NHCH(CF3)]Gly tripeptides have been studied in solution by 1H NMR spectroscopy supported by MD calcns., as well as in the solid-state by X-ray diffraction. Remarkable stability of turn-like conformations, comparable to that of parent malonyl-based retropeptides, was evidenced, as a likely consequence of two main factors: (1) severe torsional restrictions about sp3 bonds in the [CO-CH2-CH(CF3)-NH-CH(R)-CO] module, which is biased by the stereoelectronically demanding CF3 group and the R side chain and (2) formation of nine-membered intramolecularly hydrogen-bonded rings, which have been clearly detected both in CHCl3 solution and in some crystal structures. The former factor seems to be more important, as turn-like conformations were found in the solid-state even in the absence of intramol. hydrogen bonding. The relative configuration of the -C*H(CF3)NHC*H(R)- stereogenic centers has a major effect on the stability of the turn-like conformation, which seems to require a syn stereochem. X-ray diffraction and ab initio computational studies showed that the [-CH(CF3)NH-] group can be seen as a sort of hybrid between a peptide bond mimic and a proteolytic transition state analog, as it combines some of the properties of a peptidyl -CONH- group (low NH basicity, CH(CF3)-NH-CH backbone angle close to 120°, C-CF3 bond substantially isopolar with the C=O) with some others of the tetrahedral intermediate [-C(OX)(O-)NH-] involved in the protease-mediated hydrolysis reaction of a peptide bond (high electron d. on the CF3 group, tetrahedral backbone carbon).

ACCESSION NUMBER: 2003:788373 CAPLUS
DOCUMENT NUMBER: 140:5293
TITLE: Synthesis, structure and conformation of partially-modified retro- and retro-inverso ψ[NHCH(CF3)]Gly peptides
AUTHOR(S): Volonterio, Alessandro; Bellosta, Stefano; Bravin, Fabio; Bellucci, Maria Cristina; Bruche, Luca; Colombo, Giorgio; Malpezzi, Luciana; Mazzini, Stefania; Meille, Stefano V.; Meli, Massimiliano; Ramirez de Arellano, Carmen; Zanda, Matteo
CORPORATE SOURCE: Dipartimento di Chimica, Materiali ed Ingegneria Chimica "G. Natta" Politecnico di Milano, Milan, 20131, Italy
SOURCE: Chemistry--A European Journal (2003), 9(18), 4510-4522
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **627882-08-0**
RL: PRP (Properties)
(calculated structure of model partially-modified retro ψ[NHCH(CF3)]Gly

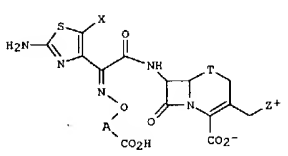
L18 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
peptides)
RN 627882-08-0 CAPLUS
CN Butanamide, 3-(methylamino)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 112 THERE ARE 112 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I

AB Cephem compds. I (T is S, SO, or O; X is halogeno, CN, carbamoyl which may be substituted with lower alkyl, lower alkyl, lower alkoxy, or lower alkylthio; A is substituted lower alkylene (wherein the substituent is optionally substituted mono-lower alkyl, optionally substituted lower alkylidene, or optionally substituted lower alkylene); and Z+ is an optionally substituted nitrogenous heterocyclic group having a cationic group), their ester, protected 7-aminothiazole, or pharmaceutically acceptable salts or solvates, are prepared I [X = Me, A = Me2C, T = S, Z = 1-(3-methylaminopropyl)-1H-imidazo[4,5-b]pyridinium-4-yl-] was prepared and showed antibacterial activities superior to that of ceftazidime.

ACCESSION NUMBER: 2003:757715 CAPLUS
DOCUMENT NUMBER: 139:261088
TITLE: Preparation of broad-spectrum cephem compounds
INVENTOR(S): Nishitani, Yasuhiro; Yamano, Yoshinori
PATENT ASSIGNEE(S): Shionogi & Co., Ltd., Japan
SOURCE: PCT Int. Appl., 209 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

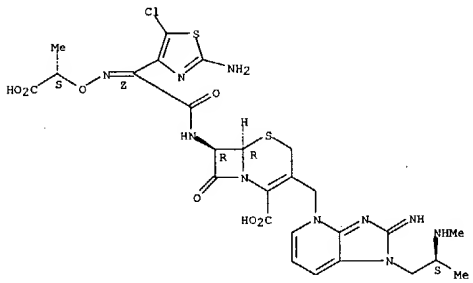
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003078440	A1	20030925	WO 2003-JP3249	20030318

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 2002-73526 A 20020318
OTHER SOURCE(S): MARPAT 139:261088
IT **604001-16-3P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological

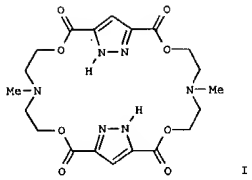
L18 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
study); PREP (Preparation); USES (Uses)
(prepn. of broad-spectrum cephem compds.)
RN 604001-16-3 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2Z)-(2-amino-5-chloro-4-thiazolyl)[[(1S)-1-carboxyethoxy]imino]acetyl]amino]-3-[[1,2-dihydro-2-imino-1-[(2S)-2-(methylamino)propyl]-4H-imidazo[4,5-b]pyridin-4-yl]methyl]-8-oxo-, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I

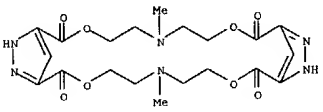
AB The equilibrium stability consts. (Ks) of a series of ammonium pyrazolate complexes [L2-2]2RN(R')H2+ (7, R' = H and 8, R' = Me, L2H2 = I) formed from a new macrocyclic disodium dipyrazolate salt of diazatetraester structure 6 [L2-2] 2Na+ and ammonium salts [RNH3+X- or RN(Me)H-2X-] of psychotropic drugs and neurotransmitter catecholamines has been evaluated by electrochem. methods in DMSO solution The resulting Ks values demonstrate that in general, the diazatetraester crown-derived dipyrazolate salt 6 exerts a stronger complexing effect over phenethylammonium ions than that of the dioxatetraester crown-derived disodium dipyrazolate salt previously reported. Interestingly, complexes formed by secondary ammonium salts of psychotropic amines [(±)-methamphetamine, (+)-methamphetamine and (±)-3,4-methylenedioxymethamphetamine (MDMA "ecstasy")] are much more stable than those formed by primary ammonium salts of dopamine and norepinephrine. A study of the stability consts. of ammonium pyrazolate complexes in terms of the contributions of substituent groups on the common phenethylamine unit is reported.

ACCESSION NUMBER: 2003:732432 CAPLUS
DOCUMENT NUMBER: 140:198977
TITLE: A new macrocyclic dipyrazolate salt of diazatetraester structure able to efficiently and selectively interact with psychotropic phenethylammonium salts: Influence of the amine substituents on the stability of the ammonium dipyrazolate complexes
AUTHOR(S): Reviriego, Felipe; Navarro, Pilar; Domenech, Antonio; Garcia-Espana, Enrique
CORPORATE SOURCE: Instituto de Quimica Medica, CSIC, Madrid, 28006, Spain
SOURCE: Journal of Supramolecular Chemistry (2003), Volume Date 2002, 2(1-3), 115-122
CODEN: JSCOC9; ISSN: 1472-7862
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **660818-62-2**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

L18 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(formation const.; selective complexation of macrocyclic diaza tetraester dipyrazolate salt receptor with psychotropic phenethylammonium salts relative to neurotransmitter catecholamines)
RN 660818-62-2 CAPLUS
CN 3,9,16,22-Tetraoxa-6,12,13,19,25,26-hexaazatricyclo[22.2.1.111,14]octacosa-1(27),11,14(28),24-tetraene-2,10,15,23-tetrone, 6,19-dimethyl-, compd. with (αS)-N,α-dimethylbenzeneethanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 219830-98-5
CMF C20 H26 N6 O8



CM 2

CRN 537-46-2
CMF C10 H15 N

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

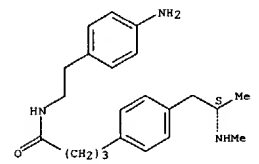
L18 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AB Compds. including haptens, intermediates, and immunogens that are useful in the production of antibodies specific for the methylenedioxy class of amphetamine derivs. are described. Antibodies specific for the methylenedioxy class of amphetamine derivs., reagent kits containing antibodies specific for the methylenedioxy class of amphetamine derivs., methods of producing antibodies specific for the methylenedioxy class of amphetamine derivs., and methods of detecting analytes including members of the methylenedioxy class of amphetamine derivs. are also described.

ACCESSION NUMBER: 2003:693232 CAPLUS
DOCUMENT NUMBER: 139:207729
TITLE: Amphetamine derivatives, antibodies to the derivatives, reagent kits, methods of producing the antibodies, and methods of detecting the derivatives
INVENTOR(S): Hui, Raymond A.; Root, Richard T.; Vitone, Stephan S.
PATENT ASSIGNEE(S): Roche Diagnostics G.m.b.H., Germany; F. Hoffmann-La Roche A.-G.
SOURCE: Eur. Pat. Appl., 34 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1340980	A1	20030903	EP 2003-3297	20030225
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2003170917	A1	20030911	US 2002-87612	20020301
JP 2004123692	A2	20040422	JP 2003-49992	20030226
PRIORITY APPLN. INFO.:			US 2002-87612 A	20020301

OTHER SOURCE(S): MARPAT 139:207729
IT **590346-44-4D**, BSA conjugates **590346-45-5D**, BSA conjugates
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(amphetamine derivs., anti-derivative antibodies, reagent kits, antibody production, and derivative detection methods)
RN 590346-44-4 CAPLUS
CN Benzenebutanamide, N-[2-(4-aminophenyl)ethyl]-4-[(2S)-2-(methylamino)propyl]- (9CI) (CA INDEX NAME)

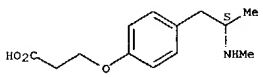
Absolute stereochemistry.



RN 590346-45-5 CAPLUS

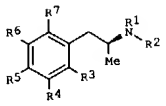
L18 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN Propanoic acid, 3-[4-[(2S)-2-(methylamino)propyl]phenoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I

AB Hapten-carrier conjugates, (S)- I [R1, R3 = H, C1-3-alkyl; R2 = H, C1-3-alkyl, polymethylene chain, (CH2)nCO2H; n = 1 - 6; R4, R6, R7 = H, halogen, OR9, SR9; R9 = H, C1-3-alkyl; R5 = H, polymethylene chain, (CH2)mR10; R10 = CO2H, SH, CONHR13SH, CONHCHR11SH; R13 = CH(CO2H)CH2, (CH2)m; m = 1 - 4, with the proviso that R1 = H, R2 = Me or R1 = Me, R2 = H and R5 = polymethylene chain, (CH2)nCO2H], capable of eliciting anti-hapten antibodies in vivo to amphetamines are disclosed. Methods of preparing the hapten-carrier conjugates and therapeutic compns. are also disclosed. A therapeutic composition containing the hapten-carrier conjugate is useful in the treatment of addiction to amphetamines. Passive immunization using antibodies raised against conjugates of the current invention is also disclosed. The therapeutic composition is suitable for co-therapy with other conventional drugs for treatment of amphetamine abuse.

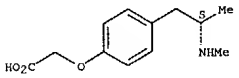
ACCESSION NUMBER: 2003:589502 CAPLUS
DOCUMENT NUMBER: 139:133711
TITLE: Preparation of new amphetamine derivatives, antibodies against them and pharmaceutical compositions containing them
INVENTOR(S): Pouletty, Philippe; Kusmierek, Jacques; Koralewski, Frederic; Galons, Herve; Blanchard, Dominique; Gadjou, Caroline; Danger, Yannic
PATENT ASSIGNEE(S): Drug Abuse Sciences, Inc., USA
SOURCE: Eur. Pat. Appl., 38 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1331219	A1	20030730	EP 2002-290169	20020123

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
PRIORITY APPLN. INFO.: EP 2002-290169 20020123
OTHER SOURCE(S): CASREACT 139:133711; MARPAT 139:133711
IT **568594-32-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

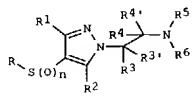
L18 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(prepn. of new amphetamine derivs., antibodies against them and pharmaceutical compns. contg. them)
RN 568594-32-1 CAPLUS
CN Acetic acid, [4-[(2S)-2-(methylamino)propyl]phenoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

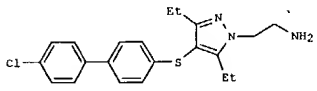


REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I



II

AB Title compds. I [n = 0-2; R = alk(en/yn)yl, aryl, etc.; R1-2 = H, OH, alkyl, alkoxy, etc.; R3, R3', R4, R4' = H, alkyl, aryl, cycloalkyl, etc.; R5-6 = H, alkyl, etc.] are prepared For instance, 4-bromothiophenol was reacted with 4-chloro-3,5-heptandione (pyridine, 3 h) and the resulting alkylation product is treated with hydrazine to give 3,5-diethyl-4-[4-bromophenyl]sulfanyl-1H-pyrazole. This intermediate is coupled to 4-chlorophenylboronic acid (PhMe, PdCl2(PPh3)2, Na2CO3, 90°, 18 h) and the product alkylated with 2-chloroethylamine to give II. Example compds. were found to have an effect on 5-HT2c receptors ≤ 10 μM. I are used for the treatment of obesity.

ACCESSION NUMBER: 2003:551498 CAPLUS
DOCUMENT NUMBER: 139:117420
TITLE: Preparation of 4-sulfanyl/sulfonyl/sulfonyl-1H-pyrazolyl compounds for use in diseases associated with the 5-HT2c receptor
INVENTOR(S): Ladouceur, Gaetan H.; Velthuisen, Emil; Choi, Soongyou; Zhang, Zhonghua; Wang, Yamin; Baryza, Jeremy L.; Coish, Philip; Smith, Roger; Chen, Michael
PATENT ASSIGNEE(S): Bayer Corporation, USA
SOURCE: PCT Int. Appl., 202 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003057674	A1	20030717	WO 2002-US41635	20021228

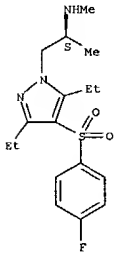
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,

L18 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.: US 2001-343749P P 20011228
OTHER SOURCE(S): MARPAT 139:117420
IT **561033-40-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(4-sulfanyl/sulfonyl/sulfonyl-1H-pyrazolyl compds. for use in diseases associated with the 5-HT2c receptor)
RN 561033-40-7 CAPLUS
CN 1H-Pyrazole-1-ethanamine, 3,5-diethyl-4-[(4-fluorophenyl)sulfonyl]-N,α-dimethyl-, (αS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 561033-39-4
CMF C17 H24 F N3 O2 S

Absolute stereochemistry.



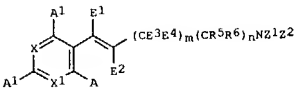
CM 2

CRN 76-05-1
CMF C2 H F3 O2

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

GI



I

AB Title compds. [I; X, X1 = N, NO, CH, CF, CCl, CBr, CI, CR', CNR'R'', CCF3, COH, CCN, CNO2, CC2R', CSH, CSMe, CN3, CSO2Me, COR', CSR', CCONR'R'', CNR'COR', CCOR', CCO2R', C(CH2)qOR', CO2CR', CO2CNR'R", CNR'CO2R', q = 1-6; A, A1, A2 = H, F, Cl, Br, iodo, R', NR'R'', CF3, OH, CN, NO2, C2R', SH, SCH3, N3, SO2CH3, OR', SR', CONR'R'', NR'COR', COR', CO2R', (CH2)qOR', O2CR', O2CNR'R" NR'CO2R'; m+n = 1-8; n ≥1; E1-E6 = H, alkyl, haloalkyl; ≥1 of E5, E6 = alkyl; Z1, Z2 = H, alkyl, COR', CO2R', CONR'R'', C(:S)R', C(:S)OR', C(:S)NR'R'', C(:NR')R', C(:NR')OR', C(:NR')NR'R"; R', R" = H, alkyl, (substituted) pyridyl, quinolinyl, pyrimidinyl, Ph, PhCH2], were prepared Thus, 3-bromopyridine, 4-penten-2-ol, palladium(II) acetate, tri-o-tolylphosphine, Et3N, and acetonitrile were heated in a sealed glass tube at 140° for 14 h. to give 81% (4E)-5-(3-pyridyl)-4-penten-2-ol. The latter was converted to the tosylate (60.1% yield) which was stirred with MeNH2 in EtOH for 18 h to give 51.6% (4E)-N-methyl-5-(3-pyridyl)-4-penten-2-amine. This in EtOH was treated with galactaric acid in 1 portion and then dropwise with H2O to give (4E)-N-methyl-5-(3-pyridyl)-4-penten-2-amine hemigalactarate. The latter showed Emax = 113% for dopamine release.

ACCESSION NUMBER: 2003:512086 CAPLUS
DOCUMENT NUMBER: 139:69159
TITLE: Preparation of pyridinylpentenylamine derivatives as nicotinic cholinergic agonists.
INVENTOR(S): Caldwell, William S.; Dull, Gary M.; Bhatti, Balwinder S.; Hadimani, Srishailkumar B.; Park, Haeil; Wagner, Jared M.; Crooks, Peter A.; Lippiello, Patrick M.; Bencherif, Merouane
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 28 pp., Cont.-in-part of U.S. Ser. No. 973,411
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 7
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003125345	A1	20030703	US 2002-263083	20021002
US 6489349	B1	20021203	US 2000-656284	20000906
US 2002052497	A1	20020502	US 2001-973411	20011009
US 2003087915	A1	20030508	US 2002-244693	20020916
WO 2004031151	A1	20040415	WO 2003-US31188	20031001

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

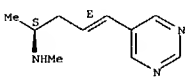
US 1996-631761	B2 19960423
US 1998-98285	B1 19980616
US 2000-522117	A1 20000309
US 2000-641496	B1 20000818
US 2001-973411	A2 20011009
US 1999-295181	A3 19990420
US 2000-570226	A1 20000512
US 2002-263083	A 20021002

OTHER SOURCE(S): MARPAT 139:69159

IT **547741-76-4P**, (S)-(4E)-N-Methyl-5-(5-pyrimidinyl)-4-penten-2-amine **552301-88-9P**, (2S)-(4E)-N-Methyl-5-(5-cyclohexyloxy-3-pyridyl)-4-penten-2-amine **552301-89-0P**, (2R)-(4E)-N-Methyl-5-(5-cyclohexyloxy-3-pyridyl)-4-penten-2-amine **552301-90-3P**, (2S)-(4E)-N-Methyl-5-(5-phenoxy-3-pyridyl)-4-penten-2-amine **552301-91-4P**, (2R)-(4E)-N-Methyl-5-(5-phenoxy-3-pyridyl)-4-penten-2-amine **552301-92-5P**, (2S)-(4E)-N-Methyl-5-[5-(4-fluorophenoxy)-3-pyridyl]-4-penten-2-amine **552301-93-6P**, (2R)-(4E)-N-Methyl-5-[5-(4-fluorophenoxy)-3-pyridyl]-4-penten-2-amine **552301-94-7P**, (2S)-(4E)-N-Methyl-5-[5-(4-chlorophenoxy)-3-pyridyl]-4-penten-2-amine **552301-95-8P**, (2R)-(4E)-N-Methyl-5-[5-(4-chlorophenoxy)-3-pyridyl]-4-penten-2-amine **552301-96-9P**, (2S)-(4E)-N-Methyl-5-[5-(3-cyanophenoxy)-3-pyridyl]-4-penten-2-amine **552301-97-0P**, (2R)-(4E)-N-Methyl-5-[5-(3-cyanophenoxy)-3-pyridyl]-4-penten-2-amine **552301-98-1P**, (2S)-(4E)-N-Methyl-5-[5-(5-indolyloxy)-3-pyridyl]-4-penten-2-amine **552301-99-2P**, (2R)-(4E)-N-Methyl-5-[5-(5-indolyloxy)-3-pyridyl]-4-penten-2-amine **552302-02-0P**, (R)-(4E)-N-Methyl-5-(5-pyrimidinyl)-4-penten-2-amine **552302-03-1P** **552302-04-2P** **552302-05-3P** **552302-06-4P** **552302-12-2DP**, (2R)-(4E)-N-Methyl-5-(5-bromo-3-pyridyl)-4-penten-2-amine, (thio)urea, (thio)carbamate, (thio)amide, amine oxide derivs. **552302-13-3DP**, (2R)-(4E)-N-Methyl-5-(5-ethoxy-3-pyridyl)-4-penten-2-amine, (thio)urea, (thio)carbamate, (thio)amide, amine oxide derivs. **552302-18-8P**, (2R)-(4E)-N-Methyl-5-(4-hydroxy-3-pyridyl)-4-penten-2-amine **552302-19-9P**, (2R)-(4E)-N-Methyl-5-(4-hydroxy-5-isopropoxy-3-pyridyl)-4-penten-2-amine **552302-22-4P**, (2S)-(4E)-N-Methyl-5-(4-hydroxy-3-pyridyl)-4-penten-2-amine **552302-24-6P**, (2S)-(4E)-N-Methyl-5-(4-hydroxy-5-isopropoxy-3-pyridyl)-4-penten-2-amine **552302-36-0P**, (2S)-(4E)-N-Methyl-5-(5-methoxy-3-pyridyl)-4-penten-2-amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyridinylpentenylamine derivs. as nicotinic cholinergic agonists)

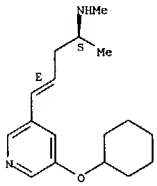
RN 547741-76-4 CAPLUS
CN 4-Penten-2-amine, N-methyl-5-(5-pyrimidinyl)-, (2S,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



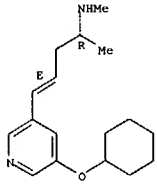
RN 552301-88-9 CAPLUS
CN 4-Penten-2-amine, 5-[5-(cyclohexyloxy)-3-pyridinyl]-N-methyl-, (2S,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



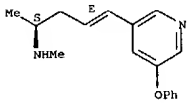
RN 552301-89-0 CAPLUS
CN 4-Penten-2-amine, 5-[5-(cyclohexyloxy)-3-pyridinyl]-N-methyl-, (2R,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



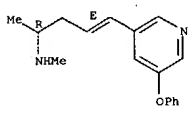
RN 552301-90-3 CAPLUS
CN 4-Penten-2-amine, N-methyl-5-(5-phenoxy-3-pyridinyl)-, (2S,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



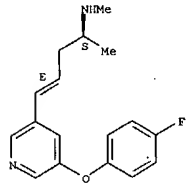
RN 552301-91-4 CAPLUS
CN 4-Penten-2-amine, N-methyl-5-(5-phenoxy-3-pyridinyl)-, (2R,4E)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



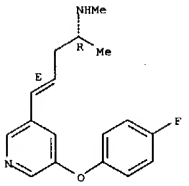
RN 552301-92-5 CAPLUS
CN 4-Penten-2-amine, 5-[5-(4-fluorophenoxy)-3-pyridinyl]-N-methyl-, (2S,4E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



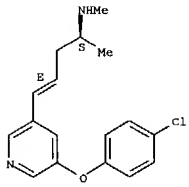
RN 552301-93-6 CAPLUS
CN 4-Penten-2-amine, 5-[5-(4-fluorophenoxy)-3-pyridinyl]-N-methyl-, (2R,4E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



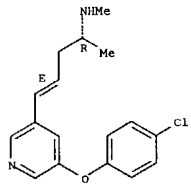
RN 552301-94-7 CAPLUS
CN 4-Penten-2-amine, 5-[5-(4-chlorophenoxy)-3-pyridinyl]-N-methyl-, (2S,4E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



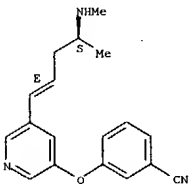
RN 552301-95-8 CAPLUS
CN 4-Penten-2-amine, 5-[5-(4-chlorophenoxy)-3-pyridinyl]-N-methyl-, (2R,4E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



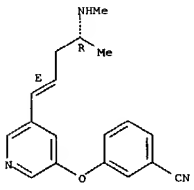
RN 552301-96-9 CAPLUS
CN Benzonitrile,
3-[[5-[(1E,4S)-4-(methylamino)-1-pentenyl]-3-pyridinyl]oxy]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



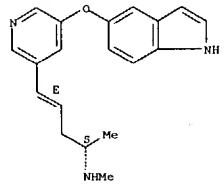
RN 552301-97-0 CAPLUS
CN Benzonitrile,
3-[[5-[(1E,4R)-4-(methylamino)-1-pentenyl]-3-pyridinyl]oxy]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



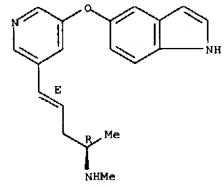
RN 552301-98-1 CAPLUS
CN 4-Penten-2-amine, 5-[5-(1H-indol-5-yloxy)-3-pyridinyl]-N-methyl-,
(2S,4E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



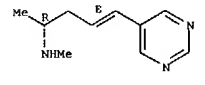
RN 552301-99-2 CAPLUS
CN 4-Penten-2-amine, 5-[5-(1H-indol-5-yloxy)-3-pyridinyl]-N-methyl-,
(2R,4E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 552302-02-0 CAPLUS
CN 4-Penten-2-amine, N-methyl-5-(5-pyrimidinyl)-, (2R,4E)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.
Double bond geometry as shown.

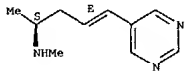


RN 552302-03-1 CAPLUS
CN Galactaric acid, compd. with
(2S,4E)-N-methyl-5-(5-pyrimidinyl)-4-penten-2-
amine (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 547741-76-4
CMF C10 H15 N3

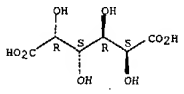
Absolute stereochemistry.
Double bond geometry as shown.



CM 2

CRN 526-99-8
CMF C6 H10 O8

Relative stereochemistry.

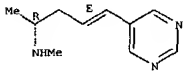


RN 552302-04-2 CAPLUS
CN Galactaric acid, compd. with (2R,4E)-N-methyl-5-(5-pyrimidinyl)-4-penten-2-amine (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 552302-02-0
CMF C10 H15 N3

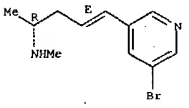
Absolute stereochemistry.
Double bond geometry as shown.



CM 2

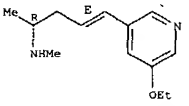
CRN 526-99-8
CMF C6 H10 O8

Relative stereochemistry.



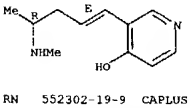
RN 552302-13-3 CAPLUS
CN 4-Penten-2-amine, 5-(5-ethoxy-3-pyridinyl)-N-methyl-, (2R,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



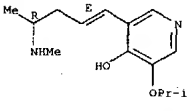
RN 552302-18-8 CAPLUS
CN 4-Pyridinol, 3-[(1E,4R)-4-(methylamino)-1-pentenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

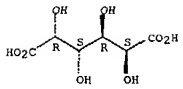


RN 552302-19-9 CAPLUS
CN 4-Pyridinol, 3-[(1E,4R)-4-(methylamino)-1-pentenyl]-5-(1-methylethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

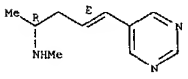


RN 552302-22-4 CAPLUS
CN 4-Pyridinol, 3-[(1E,4S)-4-(methylamino)-1-pentenyl]- (9CI) (CA INDEX NAME)



RN 552302-05-3 CAPLUS
CN 4-Penten-2-amine, N-methyl-5-(5-pyrimidinyl)-, monohydriodide, (2R,4E)- (9CI) (CA INDEX NAME)

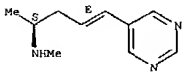
Absolute stereochemistry.
Double bond geometry as shown.



● HI

RN 552302-06-4 CAPLUS
CN 4-Penten-2-amine, N-methyl-5-(5-pyrimidinyl)-, monohydriodide, (2S,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

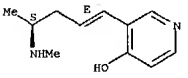


● HI

RN 552302-12-2 CAPLUS
CN 4-Penten-2-amine, 5-(5-bromo-3-pyridinyl)-N-methyl-, (2R,4E)- (9CI) (CA INDEX NAME)

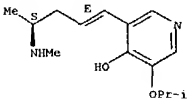
Absolute stereochemistry.
Double bond geometry as shown.

Absolute stereochemistry.
Double bond geometry as shown.



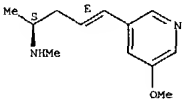
RN 552302-24-6 CAPLUS
CN 4-Pyridinol, 3-[(1E,4S)-4-(methylamino)-1-pentenyl]-5-(1-methylethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 552302-36-0 CAPLUS
CN 4-Penten-2-amine, 5-(5-methoxy-3-pyridinyl)-N-methyl-, (2S,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L18 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

AB The invention provides methods of screening for substances having an effect on a nicotine receptor by contacting a cell having a nicotine receptor with a test substance; and determining any increase or decrease in phosphorylation of Janus-Activated Kinase 2 (JAK2). An increase in phosphorylation of JAK2 indicates that the test substance stimulates the nicotine receptor, and wherein a decrease in phosphorylation of JAK2 indicates that the test substance inhibits the nicotine receptor. The invention also provides screening methods for identification of substances that affect nicotine receptor activity through activity mediated by the AT2 receptor. Related pharmaceutical compns. and methods of treatment of CNS disorders are also provided.

ACCESSION NUMBER: 2003:490993 CAPLUS
DOCUMENT NUMBER: 139:47183
TITLE: Screening methods for compounds that affect nicotine receptors and compositions for treatment of central nervous system disorders
INVENTOR(S): Bencherif, Merouane; Marrero, Mario B.
PATENT ASSIGNEE(S): Targacept, Inc., USA; Medical College of Georgia Research Institute, Inc.
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003051302	A2	20030626	WO 2002-US39952	20021213
WO 2003051302	A3	20030904		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003158211	A1	20030821	US 2002-318842	20021213

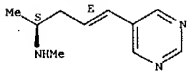
PRIORITY APPLN. INFO.: US 2001-340582P P 20011214
US 2002-369934P P 20020404

IT **547741-76-4**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(as nicotine receptor stimulant; screening methods for compds. that affect nicotine receptors and compns. for treatment of central nervous system disorders)

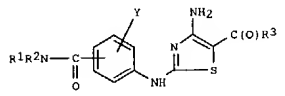
RN 547741-76-4 CAPLUS
CN 4-Penten-2-amine, N-methyl-5-(5-pyrimidinyl)-, (2S,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

L18 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L18 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I

AB Aminothiazole compds. with mono-/di-substituted benzamides (shown as I; variables described below; e.g. 4-[[4-amino-5-(2,6-difluorobenzoyl)thiazol-2-yl]amino]-N-(2-morpholin-4-ylethyl)benzamide), and their pharmaceutically acceptable salts, pharmaceutically acceptable prodrugs, pharmaceutically active metabolites, and pharmaceutically acceptable salts of said metabolites are described. These agents modulate and/or inhibit the cell proliferation and activity of protein kinases and are useful as pharmaceuticals for treating malignancies and other disorders. Inhibitory activities towards three cyclin complexes of protein kinases, phosphorylated FGF receptor and/or LCK tyrosine kinase and/or cytotoxicity towards the HCT-116 cancer cell line are reported for hundreds of I, many of which were prepared combinatorially. For I: R1 and R2 are each independently H, or an alkyl, alkenyl, alkynyl, heteroalkyl, alkoxy, aminoalkyl, aryl, heteroaryl, cycloalkyl, or heterocycloalkyl group unsubstituted or substituted with ≥1 substituents listed in the claims, or R1 or R2, together with the N-C(O) and two adjacent C atoms of the Ph ring of I, forms a 5- or 6-membered ring structure fused to the Ph ring of I and unsubstituted or substituted with ≥1 substituents listed in the claims, or R1 and R2, taken together with the N atom to which they are bonded, form a monocyclic or fused or nonfused polycyclic structure which may contain 1-3 addnl. heteroatoms, the structure being unsubstituted or substituted with ≥1 substituents listed in the claims. R3 is an aryl, heteroaryl, alkyl, or cycloalkyl group, unsubstituted or substituted with ≥1 substituents listed in the claims. Y is H, alkyl, heteroalkyl, haloalkyl, halocycloalkyl, haloheterocycloalkyl, cycloalkyl, heterocycloalkyl, -NO2, -NH2, -N-OH, N-ORc, -CN, -(CH2)z-CN (z is 0-4), halogen, -OH, -O-Ra-O-, -ORb, -CO-R, -O-CO-Rc, -CO-ORc, -O-CO-OR, -O-OR, =O, =S, -NRdRe, -CO-NRdRe, -O-CO-NRdRe, -NRc-CO-Re, -NR-CO-OR, -CO-NRc-CO-Rd, -O-SO2-Re, -O-SO-R, -O-S-Re, -S-CO-Rc, -SO-CO-ORc, -SO-CO-OR, -O-SO3, -NRc-SRd, -NRc-SO-Rd, NRc-SO2-Rd, -CO-SRc, -CO-SO-Re, -CO-OSO2-Rc, -CS-Rc, -CSO-R, -CSO2-R,, -NRc-CS-Rd, -O-CS-Re, -O-CSO-Rc, -O-SO2-Re, -OS2-NRdRe, -SO-NRdRe, -S-NRdRe, -NRd-CSO2-Rd, - NRc-CSO-Rd, -NRc-CS-Rd, -SH, -S-Rb, and -PO2-ORc (Ra, etc. defined in claims). Although the methods of preparation are not claimed, approx.80 example prepns. of I are included and directions are given for combinatorial preparation of 396 I.

ACCESSION NUMBER: 2003:42245 CAPLUS
DOCUMENT NUMBER: 138:106689
TITLE: Preparation of thiazolylamino benzamide derivatives as modulators of cell proliferation and inhibitors of protein kinases
INVENTOR(S): Chu, Shao Song; Alegria, Larry Andrew; Bleckman, Ted Michael; Chong, Wesley K. M.; Duvadie, Rohit K.; Li, Lin; Reich, Siegfried H.; Romines, William H.; Wallace, Michael B.; Yang, Yi
PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 163 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003004467	A2	20030116	WO 2002-US21280	20020705

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003225147	A1	20031204	US 2002-190219	20020705
US 6720346	B2	20040413		

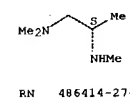
PRIORITY APPLN. INFO.: US 2001-303679P P 20010706
US 2001-305274P P 20010713

OTHER SOURCE(S): MARPAT 138:106689

IT **486414-25-9P**, (S)-N1,N1,N2-Trimethylpropane-1,2-diamine
486414-27-1P, (R)-N1,N1,N2-Trimethylpropane-1,2-diamine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of thiazolylamino benzamide derivs. as modulators of cell proliferation and inhibitors of protein kinases)

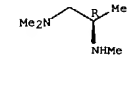
RN 486414-25-9 CAPLUS
CN 1,2-Propanediamine, N1,N1,N2-trimethyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 486414-27-1 CAPLUS
CN 1,2-Propanediamine, N1,N1,N2-trimethyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



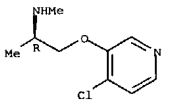
AB Analogs of the potent nicotinic receptor agonist 3-(2-aminoethoxy)pyridine substituted at the 5' and 6'-positions of the pyridine ring were synthesized and tested in vitro for nicotinic receptor binding activity (displacement of [3H](-)cytisine from whole rat brain synaptic membranes). The substituted analogs exhibited Ki values ranging from 0.076 to 319 nM compared to a Ki value of 26 nM for previously identified A-84543. Among the compds. tested, 5'-vinyl-6'-chloro substituted A-84543 was the most potent.

ACCESSION NUMBER: 2002:808837 CAPLUS
DOCUMENT NUMBER: 138:187613
TITLE: Synthesis and biological evaluation of pyridine-modified analogues of 3-(2-Aminoethoxy)pyridine as novel nicotinic receptor ligands
AUTHOR(S): Lin, Nan-Horng; Dong, Liming; Bunnelle, William H.; Anderson, David J.; Meyer, Michael D.
CORPORATE SOURCE: Pharmaceutical Products Division, Neurological and Urological Diseases Research, Abbott Laboratories, Abbott Park, IL, 60064-3500, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(22), 3321-3324
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:187613

IT **497949-17-4P 497949-18-5P 497949-19-6P 497949-20-9P 497949-21-0P 497949-22-1P 497949-23-2P 497949-24-3P 497949-25-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn of pyridine analogs of 3-(2-aminoethoxy)pyridine from α-amino carboxylic acids and evaluation of their activity as nicotinic receptor ligands)

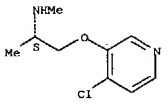
RN 497949-17-4 CAPLUS
CN 2-Propanamine, 1-[(4-chloro-3-pyridinyl)oxy]-N-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



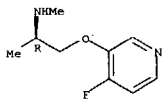
RN 497949-18-5 CAPLUS
CN 2-Propanamine, 1-[(4-chloro-3-pyridinyl)oxy]-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



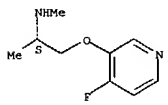
RN 497949-19-6 CAPLUS
CN 2-Propanamine, 1-[(4-fluoro-3-pyridinyl)oxy]-N-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



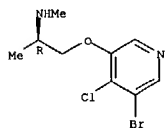
RN 497949-20-9 CAPLUS
CN 2-Propanamine, 1-[(4-fluoro-3-pyridinyl)oxy]-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 497949-21-0 CAPLUS
CN 2-Propanamine, 1-[(5-bromo-4-chloro-3-pyridinyl)oxy]-N-methyl-, (2R)- (9CI) (CA INDEX NAME)

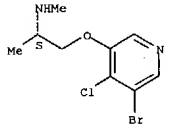
Absolute stereochemistry.



RN 497949-22-1 CAPLUS
CN 2-Propanamine, 1-[(5-bromo-4-chloro-3-pyridinyl)oxy]-N-methyl-, (2S)-

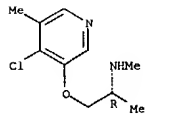
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



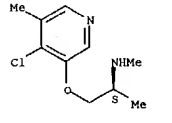
RN 497949-23-2 CAPLUS
CN 2-Propanamine, 1-[(4-chloro-5-methyl-3-pyridinyl)oxy]-N-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 497949-24-3 CAPLUS
CN 2-Propanamine, 1-[(4-chloro-5-methyl-3-pyridinyl)oxy]-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

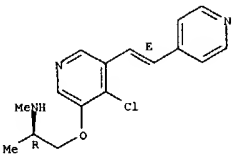
Absolute stereochemistry.



RN 497949-25-4 CAPLUS
CN 2-Propanamine, 1-[[4-chloro-5-[(1E)-2-(4-pyridinyl)ethenyl]-3-pyridinyl]oxy]-N-methyl-, (2R)- (9CI) (CA INDEX NAME)

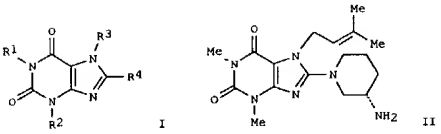
Absolute stereochemistry.
Double bond geometry as shown.

L18 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L18 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
GI



AB Xanthine derivs. of formula I [R1, R2 = H, alkyl, alkenyl, etc.; R3 = alkyl, arylalkyl, etc.; R4 = heterocyclyl, cycloalkyl, aminoalkyl, etc.] are prepared which exhibit an inhibitory effect on the activity of the dipeptidylpeptidase-IV enzyme. Pharmaceutical compns. containing I are described. Thus, II was prepared and had an IC50 of 22 nM against dipeptidylpeptidase-IV.

ACCESSION NUMBER: 2002:676018 CAPLUS
DOCUMENT NUMBER: 137:216824
TITLE: Preparation of xanthine derivatives as dipeptidylpeptidase-IV inhibitors
INVENTOR(S): Himmelsbach, Frank; Mark, Michael; Eckhardt, Matthias; Langkopf, Elke; Maier, Roland; Lotz, Ralf
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany
SOURCE: PCT Int. Appl., 373 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002068420	A1	20020906	WO 2002-EP1820	20020221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10109021	A1	20020905	DE 2001-10109021	20010224
DE 10117803	A1	20021024	DE 2001-10117803	20010410
DE 10140345	A1	20030227	DE 2001-10140345	20010817
DE 10203486	A1	20030731	DE 2002-10203486	20020130
EP 1368349	A1	20031210	EP 2002-701288	20020221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
EE 200300409	A	20031215	EE 2003-409	20020221
BR 2002007767	A	20040330	BR 2002-7767	20020221

L18 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

NO 2003003726	A	20030821	NO 2003-3726	20030821
US 2004077645	A1	20040422	US 2003-467961	20031205

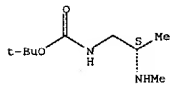
PRIORITY APPLN. INFO.: DE 2001-10109021 A 20010224
DE 2001-10117803 A 20010410
DE 2001-10140345 A 20010817
DE 2002-10203486 A 20020130
WO 2002-EP1820 W 20020221

OTHER SOURCE(S): MARPAT 137:216824

IT **454709-95-6P 454709-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of xanthine derivs. as dipeptidylpeptidase-IV inhibitors)

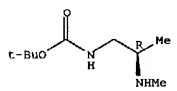
RN 454709-95-6 CAPLUS
CN Carbamic acid, [(2S)-2-(methylamino)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 454709-96-7 CAPLUS
CN Carbamic acid, [(2R)-2-(methylamino)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L18 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

AB The equilibrium stability consts. (Ks) of ammonium pyrazolate complexes {L2-}2RN(R')H2+ (3, R' = H and 4, R' = Me) formed from a macrocyclic disodium dipyrazolate salt 2{L2-} 2Na+ and ammonium salts (RNH3+X- or RN(Me)H2+X-) of psychotropic drugs and neurotransmitter catecholamines have been evaluated by electrochem. methods in DMSO solution The resulting
Ks values demonstrate that, except for (±)-amphetamine, the complexes formed by lipophilic primary [mescaline, (+)-amphetamine, (±)-p-methoxyamphetamine (PMA), (±)-3,4-methylenedioxyamphetamine (MDA)] and secondary [(±)-methamphetamine, (+)-methamphetamine and (±)-3,4-methylenedioxymethamphetamine (MDMA ecstasy')] phenethylamines are more stable than those formed from hydrophilic ones (dopamine and norepinephrine). A 1H and 13C NMR study on the formation of complexes of structure 3 and 4 formed from primary [mescaline, (+)-amphetamine] and secondary [(+)-methamphetamine] ammonium salts is given.

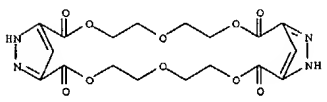
ACCESSION NUMBER: 2002:647697 CAPLUS
DOCUMENT NUMBER: 138:406723
TITLE: Effective complexation of psychotropic phenethylammonium salts from a disodium dipyrazolate salt of macrocyclic structure
AUTHOR(S): Reviriego, Felipe; Navarro, Pilar; Domenech, Antonio; Garcia-Espana, Enrique
CORPORATE SOURCE: Instituto de Quimica Medica, CSIC, Madrid, 28006, Spain
SOURCE: Journal of the Chemical Society, Perkin Transactions 2
(2002), (9), 1634-1638
CODEN: JCSPGI; ISSN: 1472-779X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **531513-34-5**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(complexation of psychotropic phenethylammonium salts from a disodium dipyrazolate salt of macrocyclic structure)

RN 531513-34-5 CAPLUS
CN 3,6,9,16,19,22-Hexaoxa-12,13,25,26-tetraazatricyclo[22.2.1.111,14]octacosa-1(27),11,14(28),24-tetraene-2,10,15,23-tetrone, compd. with (αS)-N,α-dimethylbenzeneethanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 134778-22-6
CMF C18 H20 N4 O10



L18 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CM 2

CRN 537-46-2
CMF C10 H15 N

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=>  fil reg
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STRUCTURE FILE UPDATES:     4 MAY 2004  HIGHEST RN 679784-15-7
DICTIONARY FILE UPDATES:    4 MAY 2004  HIGHEST RN 679784-15-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> s 389140-14-1/rn
L19           1 389140-14-1/RN

=> d l19
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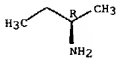
L19 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN **389140-14-1** REGISTRY
CN Benzenemethanol, α-ethyl-, (αR)-, compd. with (2R)-2-butanamine (1:1) (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C9 H12 O . C4 H11 N
SR CA
LC STN Files: CA, CAPLUS

CM 1

CRN 13250-12-9
CMF C4 H11 N

Absolute stereochemistry. Rotation (-).



CM 2

CRN 1565-74-8
CMF C9 H12 O

Absolute stereochemistry. Rotation (+).

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY     SESSION
FULL ESTIMATED COST                                    5.13      714.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY     SESSION
CA SUBSCRIBER PRICE                                    0.00      -56.14

FILE 'CAPLUS' ENTERED AT 17:03:15 ON 05 MAY 2004
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```



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FILE COVERS 1907 - 5 May 2004  VOL 140 ISS 19
FILE LAST UPDATED: 4 May 2004  (20040504/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s 389140-14-1/rn
             1 389140-14-1
             0 389140-14-1D
L20          1 389140-14-1/RN
                 (389140-14-1 (NOTL) 389140-14-1D )

=> d l20 abs ibib hitstr
```

L20 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

AB A methodol. has been developed for enantiodiscriminating chiral monoalcs. and monoamines by mass spectrometry. The approach is based on the generation of supersonically expanded complexes of these mols. with suitable chromophores, i.e. R-(+)-1-phenyl-ethanol (ER) or R-(+)-1-phenyl-1-propanol (PR). The jet-cooled diastereomeric complexes, otherwise elusive at room temperature, have been ionized by one-color resonant two-photon absorption (R2PI) and their fragmentation pattern analyzed by time-of-flight (TOF) spectrometry. Enantiodifferentiation of the chiral monoalcs. and monoamines is based on: (1) the different spectral shifts of the band origin of their mol. complexes relative to that of the bare chromophore (A) and (2) the different mass spectral fragmentation patterns of the jet-cooled diastereomeric adducts. Detection of stable aggregates of methane, n-butane, and other simple mols. with the selected chromophores suggests that the R2PI/TOF method can be a potential tool for enantiodifferentiating chiral hydrocarbons in the gas phase.

ACCESSION NUMBER: 2001:746816 CAPLUS
DOCUMENT NUMBER: 136:134373
TITLE: Chiral discrimination of monofunctional alcohols and amines in the gas phase
AUTHOR(S): Filippi, A.; Giardini, A.; Latini, A.; Piccirillo, S.; Scuderi, D.; Speranza, M.
CORPORATE SOURCE: Dipartimento di Studi di Chimica e Tecnologia delle Sostanze Biologicamente Attive, Universita di Roma "La Sapienza", Rome, 00185, Italy
SOURCE: International Journal of Mass Spectrometry (2001), 210/211(1-3), 483-488
CODEN: IMSPF8; ISSN: 1387-3806
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

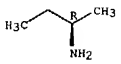
IT **389140-14-1**
RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(R2PI/TOF method for enantiodifferentiating chiral hydrocarbons in gas phase)

RN 389140-14-1 CAPLUS
CN Benzenemethanol, α-ethyl-, (αR)-, compd. with (2R)-2-butanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 13250-12-9
CMF C4 H11 N

Absolute stereochemistry. Rotation (-).



CM 2

CRN 1565-74-8
CMF C9 H12 O

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
=> fil reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                          ENTRY     SESSION
FULL ESTIMATED COST                                        14.08      729.06

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)              SINCE FILE      TOTAL
                                                          ENTRY     SESSION
CA SUBSCRIBER PRICE                                        -0.69      -56.83

FILE 'REGISTRY' ENTERED AT 17:11:01 ON 05 MAY 2004
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     4 MAY 2004  HIGHEST RN 679784-15-7
DICTIONARY FILE UPDATES:    4 MAY 2004  HIGHEST RN 679784-15-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\09857465.str
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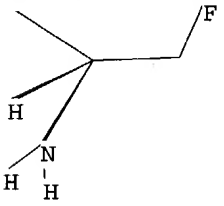

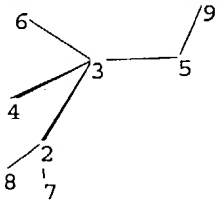


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chain nodes :
2  3  4  5  6  7  8  9
chain bonds :
2-3  2-7  2-8  3-4  3-5  3-6  5-9
exact/norm bonds :
2-3
exact bonds :
2-7  2-8  3-4  3-5  3-6  5-9


G1:H,F

Match level :
2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:CLASS  9:CLASS

Stereo Bonds:
```

3-2 (Single Wedge).
4-3 (Single Hash).

Stereo Chiral Centers:

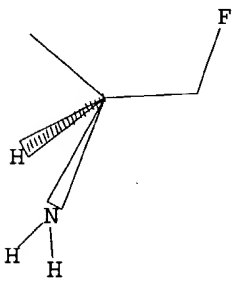
3 (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 3

L21 STRUCTURE UPLOADED

=> d query
L21 STR



G1 H,F

Structure attributes must be viewed using STN Express query preparation.

=> s l21
SAMPLE SEARCH INITIATED 17:11:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1391 TO ITERATE

71.9% PROCESSED 1000 ITERATIONS 10 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 25583 TO 30057
PROJECTED ANSWERS: 55 TO 501

L22 10 SEA SSS SAM L21

=> s l21 full
FULL SEARCH INITIATED 17:11:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 27574 TO ITERATE

100.0% PROCESSED 27574 ITERATIONS 465 ANSWERS
SEARCH TIME: 00.00.01

L23 465 SEA SSS FUL L21

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	884.48

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-56.83

FILE 'CAPLUS' ENTERED AT 17:11:26 ON 05 MAY 2004
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FILE COVERS 1907 - 5 May 2004 VOL 140 ISS 19
FILE LAST UPDATED: 4 May 2004 (20040504/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l23
L24 334 L23

=> d l24 300-334 abs ibib hitstr

L24 ANSWER 300 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN

AB The title compds. were resolved by treating with (Ac)2CH2 (I) and resolving the resulting N-(1-methyl-2-acetylvinyl) derivs. with quinine. Thus, 3-fluoro-DL-alanine (DL-II) was treated with I and quinine in MeOH for 60 min to give a crystallization quinine salt of L-AcCH:CMeNHCH(CH2F)CO2H. The latter was neutralized with 1N NaOH and the N-vinyl group was cleaved with HOAc/HCl to give 52.4% L-II. D-II (45%) was obtained from the filtrates and washings of the workup.

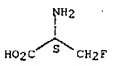
ACCESSION NUMBER: 1977:584966 CAPLUS
DOCUMENT NUMBER: 87:184966
TITLE: Resolving alanine, 3-fluoro- and 2-deutero-3-fluoro-DL-alanine
INVENTOR(S): Chemerda, John M.; Gal, George
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4048224	A	19770913	US 1976-664328	19760305
FI 7700493	A	19770906	FI 1977-493	19770215
SE 7701710	A	19770906	SE 1977-1710	19770216
DK 7700674	A	19770906	DK 1977-674	19770216
NL 7701643	A	19770907	NL 1977-1643	19770216
NO 7700524	A	19770906	NO 1977-524	19770217
CS 195327	P	19800131	CS 1977-1133	19770221
SU 786887	D	19801207	SU 1977-2454448	19770222
AT 348501	B	19790226	AT 1977-1382	19770302
JP 52106814	A2	19770907	JP 1977-22281	19770303
PL 105883	P	19791130	PL 1977-196414	19770303
HU 172989	P	19790128	HU 1977-ME2047	19770304

PRIORITY APPLN. INFO.: US 1976-664328 19760305

IT **35455-20-0P 35455-21-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by resolution of 3-fluoro-DL-alanine)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

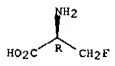
Absolute stereochemistry. Rotation (-).



RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

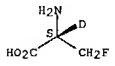
Absolute stereochemistry.

L24 ANSWER 300 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



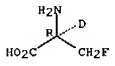
IT **35523-45-6P 59189-05-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from resolution of racemic compound)
RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 59189-05-8 CAPLUS
CN L-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



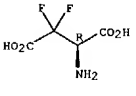
L24 ANSWER 301 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN

AB Fluorination of di-tert-Bu oxaloacetate [64336-61-4] followed by oximation, reduction, and hydrolysis gave dl-β,β-difluoroaspartic acid (dl-I) [64336-65-8] which was resolved via its brucine salts. Dl-I was selectively esterified and treated with NH3-MeOH to give β,β-difluoroasparagine [64336-67-0]. Conversion of aspartate into oxaloacetate, catalyzed by aspartate aminotransferase (EC 2.6.1.1) [9000-97-9], was competitively inhibited by dl-I. Cell growth of 3T3-F cells in culture was slightly inhibited by l-I NH4 salt [**64336-69-2**], but not by d-I NH4 salt [**64336-70-5**]. In vivo L-5178Y lymphatic leukemia was unaffected by dl-I or difluoroasparagine in nontoxic doses.

ACCESSION NUMBER: 1977:577664 CAPLUS
DOCUMENT NUMBER: 87:177664
TITLE: Potential carcinostatics. Synthesis and biological properties of d- and l-β,β-difluoroaspartic acid and β,β-difluoroasparagine
AUTHOR(S): Hageman, Johanna J. M.; Wanner, Martinus J.; Koomen, Gerrit Jan; Pandit, Upendra K.
CORPORATE SOURCE: Org. Chem. Lab., Univ. Amsterdam, Amsterdam, Neth.
SOURCE: Journal of Medicinal Chemistry (1977), 20(12), 1677-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **64336-69-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and neoplasm inhibiting activity of)
RN 64336-69-2 CAPLUS
CN L-Aspartic acid, 3,3-difluoro-, monoammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

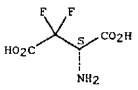


● NH_3

IT **64336-70-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as neoplasm inhibitor)
RN 64336-70-5 CAPLUS
CN D-Aspartic acid, 3,3-difluoro-, monoammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L24 ANSWER 301 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



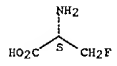
● NH_3

L24 ANSWER 302 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB Alcs. were dehydroxylated-fluorinated with SF4-HF. Thus PhCHFCHMeNHMe was
obtained quant. by treating 10 mmols ephedrine in 20 mL HF with 21 mmols SF4 in a CO2-acetone bath. Other alcs. dehydroxylated-fluorintated included serine, kinin, pyridoxamine, and thiamine.
ACCESSION NUMBER: 1977:517140 CAPLUS
DOCUMENT NUMBER: 87:117140
TITLE: Fluorodehydroxylation of alcohols
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Neth. Appl., 17 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 7605557	A	19761214	NL 1976-5557	19760524
FI 7601457	A	19761213	FI 1976-1457	19760524
SE 7605910	A	19761213	SE 1976-5910	19760525
DK 7602299	A	19761213	DK 1976-2299	19760525
NO 7601796	A	19761214	NO 1976-1796	19760526
ES 448509	A1	19770701	ES 1976-448509	19760603
CH 621103	A	19810115	CH 1976-7067	19760603
CA 1063617	A1	19791002	CA 1976-254108	19760604
JP 51149208	A2	19761222	JP 1976-67862	19760611
JP 60033808	B4	19850805		

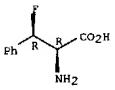
PRIORITY APPLN. INFO.: US 1975-586326 19750612
IT **35455-20-0P 76582-46-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 76582-46-2 CAPLUS
CN Phenylalanine, β-fluoro-, threo- (9CI) (CA INDEX NAME)

Relative stereochemistry.

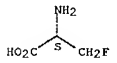


L24 ANSWER 303 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB 3-Fluoro-D-alanine **[35455-20-0]** and D-cycloserine [68-41-7] were each capable of protecting mice against infections with various bacteria, but synergistic effects of combinations resulted in equivalent levels of protection at drug concns. of only 5-10% of those required when they were used individually. In addition, concns. of D-cycloserine providing zero protection were capable of reversing the autoantagonism occurring with high concns. of fluoroalanine. If not blocked by cycloserine, this latter
effect resulted in a lesser degree of protection from a 5 mg dose of fluoroalanine than from a 1.25 mg dose.
ACCESSION NUMBER: 1977:496261 CAPLUS
DOCUMENT NUMBER: 87:96261
TITLE: Antibacterial composition comprising 3-fluoro-D-alanine or deutero analog in combination with auto-antagonist inhibitor
INVENTOR(S): Kahan, Frederick M.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4031231	A	19770621	US 1976-651878	19760123
AU 7351368	A1	19740725	AU 1973-51368	19730123
ZA 7300761	A	19740925	ZA 1973-761	19730202
ZA 7404366	A	19750730	ZA 1974-4366	19740708
BE 818335	A4	19750131	BE 1974-147155	19740731

PRIORITY APPLN. INFO.: US 1972-223360 19720203
US 1972-314878 19721213
US 1973-387571 19730810
US 1974-478793 19740613
IT **35455-20-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(antibacterial activity of, in infection, cycloserine synergistic effect on)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



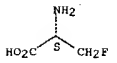
L24 ANSWER 304 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB Organic compds. having one or more replaceable H atoms are fluorinated in the
liquid or solid state by treatment with fluoroxyperfluoroalkanes or FOSF5 under free radical conditions. The method was applied to a large variety of substrates, e.g., mono- or polynuclear aromatic or alicyclic compds. Thus, a cooled solution of C6H6 in FCCl3 is irradiated with UV light and treated with FOCF3(g) for 1 h to give 65% PhF.
ACCESSION NUMBER: 1977:483904 CAPLUS
DOCUMENT NUMBER: 87:83904
TITLE: Substitutive fluorination of organic compounds
INVENTOR(S): Kollonitsch, Janos
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4030994	A	19770621	US 1973-404555	19731009
NL 7109946	A	19720207	NL 1971-9946	19710719
NL 173388	B	19830816		
NL 173388	C	19840116		
AU 7131463	A1	19730125	AU 1971-31463	19710720
CA 967982	A1	19750520	CA 1971-118803	19710721
IT 988052	A	19750410	IT 1971-51835	19710722
GB 1353519	A	19740522	GB 1971-34887	19710726
FR 2101198	A5	19720331	FR 1971-28394	19710803
FR 2101198	B1	19750801		
FR 2103901	A5	19720414	FR 1971-28393	19710803
ZA 7105185	A	19730328	ZA 1971-5185	19710803
HU 163751	P	19731027	HU 1971-ME1404	19710803
HU 166452	P	19750328	HU 1971-ME1550	19710803
CH 575354	A	19760514	CH 1971-11408	19710803
JP 55044048	B4	19801110	JP 1971-58028	19710803
FR 2142474	A5	19730126	FR 1972-21616	19720615
CA 968368	A2	19750527	CA 1974-205439	19740723
CA 994360	A2	19760803	CA 1974-210939	19741008
AT 7408827	A	19760315	AT 1974-8827	19741104
AT 333246	B	19761110		

PRIORITY APPLN. INFO.: US 1970-60645 19700803
US 1971-154695 19710618
CA 1971-118803 19710721
US 1972-223354 19720203
CA 1972-144614 19720613
AT 1972-5115 19720614
IT **35455-20-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

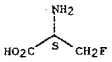
Absolute stereochemistry. Rotation (-).

L24 ANSWER 304 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L24 ANSWER 305 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB In contrast to group A streptococci or Streptococcus pneumoniae, cells of S. sanguis (group H) did not exhibit the irreversible effects of benzylpenicillin [61-33-6] treatment, such as loss of viability or lysis. On the other hand, the same bacteria showed typical effects of penicillin, such as morphological alterations reduction in the rate of cell wall synthesis, and secretion of murein and lipoteischoic acid polymers into the medium. A novel effect of cell wall inhibitors was also noted: treatment with β-lactams caused the release of substantial amts. of glycerol lipids into the growth medium. The antibiotic tolerance of S. sanguis was interpreted in terms of the hypothesis that the activity of bacterial murein hydrolases is essential for the irreversible effects of cell wall inhibitors.
ACCESSION NUMBER: 1977:478967 CAPLUS
DOCUMENT NUMBER: 87:78967
TITLE: Tolerant response of Streptococcus sanguis to beta-lactams and other cell wall inhibitors
AUTHOR(S): Horne, Diane; Tomasz, Alexander
CORPORATE SOURCE: Rockefeller Univ., New York, NY, USA
SOURCE: Antimicrobial Agents and Chemotherapy (1977), 11(5), 888-96
CODEN: AMACCQ; ISSN: 0066-4804
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **35455-20-0**
RL: PRP (Properties)
(lipids of Streptococcus sanguis response to, cell wall formation in relation to)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

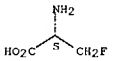


L24 ANSWER 306 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB Antibacterial deuterated 3-fluoro-D-alanines were prepared by direct photofluorination of the corresponding deuterated D-alanine. Thus, alanine was treated with alanine racemase in D2O to give D-alanine-2-d, which was fluorinated with FOCF3 in HF in the presence of UV light to give 3-fluoro-D-alanine-2-d. 3-Fluoro-D-alanine and its L-isomer were also prepared by the photofluorination of D- and L-alanine. The D-isomers of deuterated fluoroalanines exhibit both in vivo and in vitro antibacterial activity.
ACCESSION NUMBER: 1977:468655 CAPLUS
DOCUMENT NUMBER: 87:68655
TITLE: Fluorinated amino acids
INVENTOR(S): Kollonitsch, Janos; Kahan, Frederick M.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4028405	A	19770607	US 1976-693819	19760607
PRIORITY APPLN. INFO.:			US 1971-149814	19710603
			US 1972-238684	19720327
			US 1974-514865	19741015

IT **39621-34-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and neutralization of)
RN 39621-34-6 CAPLUS
CN D-Alanine, 3-fluoro-, hydrochloride (9CI) (CA INDEX NAME)

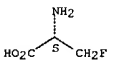
Absolute stereochemistry. Rotation (-).



● HCl

IT **35455-20-0P 35455-21-1P 35523-45-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

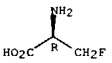
Absolute stereochemistry. Rotation (-).



L24 ANSWER 306 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

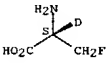
RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



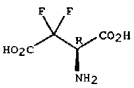
RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 307 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB Difluorooxalacetate behaved as a competitive inhibitor of 2-oxoglutarate and as a noncompetitive inhibitor with resp. to aspartate in steady-state kinetic expts. with pig heart cytoplasmic aspartate aminotransferase (EC 2.6.1.1) (I). In the presence of high concns. of I difluorooxalacetate was slowly transamidated to difluoroaspartate, suggesting its use as a kinetic probe to study the aminic forms of I.
ACCESSION NUMBER: 1977:417969 CAPLUS
DOCUMENT NUMBER: 87:17969
TITLE: Interaction of difluorooxaloacetate with aspartate transaminase
AUTHOR(S): Briley, Patricia A.; Eisenthal, Robert; Harrison, Roger; Smith, Geoffrey D.
CORPORATE SOURCE: Sch. Biol. Sci., Univ. Bath, Bath, UK
SOURCE: Biochemical Journal (1977), 161(2), 383-7
CODEN: BIJOAK; ISSN: 0264-6021
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **63086-45-3**
RL: FORM (Formation, nonpreparative)
(formation of, from difluorooxalacetate, by aspartate aminotransferase)
RN 63086-45-3 CAPLUS
CN L-Aspartic acid, 3,3-difluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 308 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB Antibacterial D-H2NCH(CH2F)CO2H (D-I) was prepared from DL-I by resolving DL-PhCH2O2CNHCH(CH2F)CO2H (DL-II). Thus, DL-I was treated with PhCH2O2CCl to give DL-II which was treated with l-PhCHMeNH2 (III) to give crystalline D-II.III. The latter was acidified at pH 2 to give D-II which was hydrogenated over Pd-C to give D-I. The antibacterial activities of D-I against 7 bacteria were compared with that of D-cycloserine, tetracycline, and chloramphenicol.

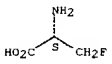
ACCESSION NUMBER: 1977:155968 CAPLUS
DOCUMENT NUMBER: 86:155968
TITLE: 3-Fluoro-D-alanine, 2-deutero-3-fluoro-D-alanine, or 2,3,3-trideutero-3-fluoro-D-alanine
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Austrian, 6 pp. Division of Austrian 322,524.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 332859	B	19761025	AT 1974-3124	19740416
AT 7403124	A	19760215		
AT 322524	B	19750526	AT 1971-10813	19711216

PRIORITY APPLN. INFO.: AT 1971-10813 19711216

IT **35455-20-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antibiotic activity of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L24 ANSWER 309 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB Antibacterial D-CH2FCR(NH2)CO2H (I, R = H, D) were prepared by an asymmetric reduction of D-CH2FC(:NCHMePh)CO2H.D-H2NCHMePh (II). Thus, D-H2NCHMePh was treated with CH2FCOCO2H to give II which was hydrogenated over Pd-C to give D,D-CH2FCR(NHCHMePh)CO2H (III, R = H) whose further hydrogenation over Pd/C gave I·(R = H). II was deuterated over Pd-C to give III (R = D) which was hydrogenated over Pd/C to give I (R = D).

ACCESSION NUMBER: 1977:121774 CAPLUS
DOCUMENT NUMBER: 86:121774
TITLE: 3-Fluoro-D-alanine and its deutero analogs
INVENTOR(S): Reinhold, Donald F.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 4 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

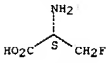
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3976689	A	19760824	US 1974-525708	19741120
NL 7300577	A	19730807	NL 1973-577	19730115
CS 178418	P	19770915	CS 1973-478	19730122
AU 7351369	A1	19740725	AU 1973-51369	19730123
CA 1001652	A1	19761214	CA 1973-161915	19730124
AT 324294	B	19750825	AT 1973-790	19730130
ES 411143	A1	19751201	ES 1973-411143	19730131
PL 84511	P	19760430	PL 1973-160498	19730131
DD 108522	C	19740920	DD 1973-168612	19730201
GB 1380382	A	19750115	GB 1973-5087	19730201
DD 114594	C	19750812	DD 1973-181401	19730201
JP 48085524	A2	19731113	JP 1973-13024	19730202
ZA 7300777	A	19741030	ZA 1973-777	19730202
SU 485592	D	19750925	SU 1973-1878868	19730202
HU 168659	P	19760628	HU 1973-ME1599	19730202
CH 585694	A	19770315	CH 1973-1489	19730202
FR 2197859	A1	19740329	FR 1973-35004	19731001
NO 7503750	A	19760521	NO 1975-3750	19751110
NL 7513137	A	19760524	NL 1975-13137	19751110
FI 7503167	A	19760521	FI 1975-3167	19751111
CH 619685	A	19801015	CH 1975-14590	19751111
SE 7512699	A	19760521	SE 1975-12699	19751112
DK 7505155	A	19760521	DK 1975-5155	19751114
DD 124972	C	19770323	DD 1975-189536	19751118
ES 442779	A1	19770916	ES 1975-442779	19751118
JP 51075020	A2	19760629	JP 1975-138818	19751120

PRIORITY APPLN. INFO.: US 1972-223355 19720203
US 1974-525708 19741120

IT **35455-20-0P 35523-45-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

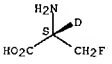
Absolute stereochemistry. Rotation (-).

L24 ANSWER 309 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



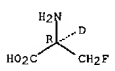
L24 ANSWER 310 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB 3-Fluoro-DL-alanine-2-d and its unlabeled analog were resolved by preparing the highly acid labile N-(1-methyl-2-acetylvinyl) amino acids as the quinine salts, and separating the diastereomers by crystallization.

ACCESSION NUMBER: 1977:55679 CAPLUS
DOCUMENT NUMBER: 86:55679
TITLE: A new and simple method of resolution. Preparation of 3-fluoro-D-alanine-2-d
AUTHOR(S): Gal, George; Chemerda, John M.; Reinhold, Donald F.; Purick, Robert M.
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Merck and Co., Inc., Rahway, NJ, USA
SOURCE: Journal of Organic Chemistry (1977), 42(1), 142-3
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **61042-77-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and acidification of)
RN 61042-77-1 CAPLUS
CN L-Alanine-2-d, 3-fluoro-, compd. with (8α,9R)-6'-methoxycinchonan-9-ol (9CI) (CA INDEX NAME)

CM 1

CRN 59189-05-8
CMF C3 H5 D F N O2

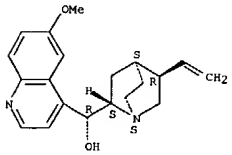
Absolute stereochemistry.



CM 2

CRN 130-95-0
CMF C20 H24 N2 O2

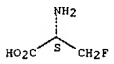
Absolute stereochemistry.



IT **35455-20-0P 35455-21-1P 35523-45-6P**

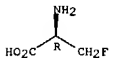
L24 ANSWER 310 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



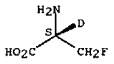
RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



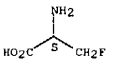
L24 ANSWER 311 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L24 ANSWER 311 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB The carbon atoms in amines, amino acids, polyamides, and vinyl polymers are fluorinated by dissolving or suspending the substrate in liquid HF, optionally containing BF3 or SbF5, at -80 to +15° and treating with F optionally under UV radiation. Thus, 5 mL liquid BF3 was added as a gas to 0.377 g D-alanine [338-69-2] in 30 mL HF at -78°, and the mixture was then treated with gaseous F as a 2% volume mixture with He for 2 h at -78° with UV irradiation, giving 3-fluoro-D-alanine [**35455-20-0**]. Other compds. fluorinated included putrescine [110-60-1], spermine [71-44-3], and polycaprolactam [25038-54-4].
ACCESSION NUMBER: 1977:44236 CAPLUS
DOCUMENT NUMBER: 86:44236
TITLE: Fluorination of organic compounds
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Neth. Appl., 15 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 7514240	A	19760625	NL 1975-14240	19751205
US 4004996	A	19770125	US 1974-535878	19741223
SE 7513572	A	19760624	SE 1975-13572	19751202
FI 7503406	A	19760624	FI 1975-3406	19751203
DK 7505502	A	19760624	DK 1975-5502	19751205
NO 7504154	A	19760624	NO 1975-4154	19751209
PL 102457	P	19790331	PL 1975-185738	19751220
JP 51088901	A2	19760804	JP 1975-152939	19751223
ES 443836	A1	19770801	ES 1975-443836	19751223

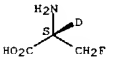
PRIORITY APPLN. INFO.: US 1974-535878 19741223
IT **35455-20-0P 35523-45-6P**
RL: PREP (Preparation)
(preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



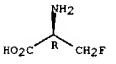
RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



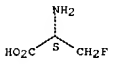
L24 ANSWER 312 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB A complementary approach to the calcn. of conformation of charged species, i.e. histamine, 2-fluoro-β-alanin, and 3-fluoro-L-alanine, in which a counter-ion is attached at an appropriate point and the wave function of the resulting neutral ion-pair is evaluated was used to determine the energies of the rotamers with CNDO MO calcns. The effects of the counter ions were also determined
ACCESSION NUMBER: 1976:577920 CAPLUS
DOCUMENT NUMBER: 85:177920
TITLE: Approaches to the problem of solvation calculations in polar and charged molecules
AUTHOR(S): Abraham, R. J.
CORPORATE SOURCE: Robert Robinson Lab., Univ. Liverpool, Liverpool, UK
SOURCE: Jerusalem Symposia on Quantum Chemistry and Biochemistry (1976), Volume Date 1975, 8(Environ. Eff. Mol. Struct. Prop.), 41-53
CODEN: JSQCA7; ISSN: 0075-3696
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **35455-21-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(solvation calcns. of, rotamer energy from)
RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 313 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB DL-β-bromoalanine-HBr was prepared from DL-β-chloroalanine-HCl and shown to be a good substrate for pig kidney D-amino acid oxidase, undergoing the O-independent elimination of HBr exclusively. D-fluoroalanine, however, undergoes only the normal oxidation reaction to fluoropyruvate.
ACCESSION NUMBER: 1976:573369 CAPLUS
DOCUMENT NUMBER: 85:173369
TITLE: Reactions of β-fluoroalanine and β-bromoalanine with D-amino acid oxidase
AUTHOR(S): Dang, Tze-Yu; Cheung, Yak-Fa; Walsh, Christopher
CORPORATE SOURCE: Dep. Chem. Biol., Massachusetts Inst. Technol., Cambridge, MA, USA
SOURCE: Biochemical and Biophysical Research Communications (1976), 72(3), 960-8
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **35455-20-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amino acid oxidase)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L24 ANSWER 314 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB 3-Fluoro-D-alanine, useful against gram-neg. and gram pos. bacteria (no data), was prepared in 41% yield by treatment of D-alanine with F3COF(g) in liquid HF for 1 hr. Esterification gave the corresponding methyl and benzyl esters.
ACCESSION NUMBER: 1976:560526 CAPLUS
DOCUMENT NUMBER: 85:160526
TITLE: 3-Fluoro-D-alanine and pharmacologically acceptable esters, and pharmacologically acceptable salts
INVENTOR(S): Kollonitsch, Janos
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 4 pp. Continuation-in-part of U.S. 3,839,170.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

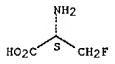
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3956367	A	19760511	US 1974-494945	19740805
FR 2101198	A5	19720331	FR 1971-28394	19710803
FR 2101198	B1	19750801		
FR 2103901	A5	19720414	FR 1971-28393	19710803
ZA 7105185	A	19730328	ZA 1971-5185	19710803
HU 166452	P	19750328	HU 1971-ME1550	19710803
US 3839170	A	19741001	US 1972-245288	19720418
PL 90080	P	19761231	PL 1972-156081	19720615
CA 968368	A2	19750527	CA 1974-205439	19740723
CA 994360	A2	19760803	CA 1974-210939	19741008
AT 7408827	A	19760315	AT 1974-8827	19741104
AT 333246	B	19761110		
AT 7502890	A	19760815	AT 1975-2890	19750416
AT 335992	B	19770412		

PRIORITY APPLN. INFO.:

US 1970-60645	19700803
US 1972-223354	19720203
US 1972-245288	19720418
US 1971-154695	19710618
CA 1971-118803	19710721
CA 1972-144614	19720613
AT 1972-5115	19720614

IT **35455-20-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

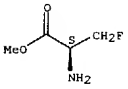
Absolute stereochemistry. Rotation (-).



IT **60644-02-2P 60644-03-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)

L24 ANSWER 314 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(prepn. of)
RN 60644-02-2 CAPLUS
CN D-Alanine, 3-fluoro-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



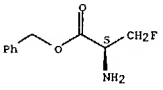
● HCl

RN 60644-03-3 CAPLUS
CN D-Alanine, 3-fluoro-, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

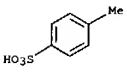
CRN 46344-20-1
CMF C10 H12 F N O2

Absolute stereochemistry.



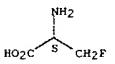
CM 2

CRN 104-15-4
CMF C7 H8 O3 S



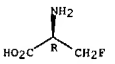
L24 ANSWER 315 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB The antibacterials 3-fluoro-D-alanine (I) and its 2-deuterated version (II) were prepared The design of I exploits a fundamental divergence in biosynthesis of the peptidoglycan component of the bacterial cell wall and of the metabolic pathways in humans. This divergence suggested application of the concept of antimetabolite synthesis via the specific approach of photofluorination. Thus, photofluorination of(D-alanine generated I which displays a high degree of antibacterial activity. A variant of I increased metabolic stability-and with unimpaired antibacterial activity-was obtained via photofluorination of 2-deuterio-D-alanine, namely 3-fluoro-D-alanine-2d (II), effective in vitro and in vivo against every bacterial strain tested.
ACCESSION NUMBER: 1976:543444 CAPLUS
DOCUMENT NUMBER: 85:143444
TITLE: Organofluorine synthesis via photofluorination: 3-fluoro-D-alanine and 2-deuterio analog, antibacterials related to the bacterial cell wall
AUTHOR(S): Kollonitsch, J.; Barash, L.
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Div., Merck and Co., Inc., Rahway, NJ, USA
SOURCE: Journal of the American Chemical Society (1976), 98(18), 5591-3
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **35455-20-0P 35455-21-1P 35523-45-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

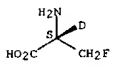
Absolute stereochemistry.



RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L24 ANSWER 315 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

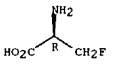


L24 ANSWER 316 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN

AB The reactions of 2-aminothiols and thiol amino acids in liquid HF solution with either FOCF3, Cl, N-chlorosuccinimide, or a fluorine-helium mixture are described. The cleavage of the C-S cond with concomitant formation of a C-F bond is observed, giving aminoalkyl fluorides and fluoro amino acids. D-penicillamine (1) was converted to D-3-fluorovaline (2) in near quant. yield while other amino thiols, following more complex pathways, furnish lower yields of the resp. fluoroproducts. The proposed mechanisms involve dihalosulfonium salts or trifluorosulfur dications which should be very good leaving groups, reacting with HF, either in a unimol. sense as in the case of penicillamine, or possibly via a bimol. mode, as in the case of cysteine. In either case, the solvent appears to be the source of fluorine in the C-F bond. A carbocation-type conversion of some alcs. to thiols was effected by reacting the appropriate alcs. with H2S in liquid HF.

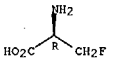
ACCESSION NUMBER: 1976:524325 CAPLUS
DOCUMENT NUMBER: 85:124325
TITLE: Fluorodesulfurization. A new reaction for the formation of carbon-fluorine bonds
AUTHOR(S): Kollonitsch, J.; Marburg, S.; Perkins, Leroy M.
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Div., Merck and Co., Inc., Rahway, NJ, USA
SOURCE: Journal of Organic Chemistry (1976), 41(19), 3107-11
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 85:124325
IT **35455-21-1P 59729-22-5P 59729-23-6P 59752-73-7P 59752-74-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 59729-22-5 CAPLUS
CN L-Alanine, 3-fluoro-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

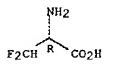


● HCl

L24 ANSWER 316 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

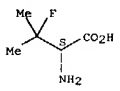
RN 59729-23-6 CAPLUS
CN L-Alanine, 3,3-difluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 59752-73-7 CAPLUS
CN D-Valine, 3-fluoro-, hydrochloride (9CI) (CA INDEX NAME)

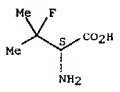
Absolute stereochemistry.



● HCl

RN 59752-74-8 CAPLUS
CN D-Valine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 317 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN

AB Treatment of 3-fluoro-L-alanine with 6N HBr and NaNO2 gave L-2-bromo-3-fluoropropionic acid which reacted with liquid NH3 in a bomb for 5 days to give 3-fluoro-D-alanine, useful as a bactericide (no data). Similarly, 2-deutero-3-fluoro-L-alanine, prepared from EtO2CCOCHFCO2Et, gave 2-deutero-3-fluoro-D-alanine.

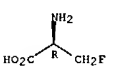
ACCESSION NUMBER: 1976:447053 CAPLUS
DOCUMENT NUMBER: 85:47053
TITLE: Asymmetric conversion of 3-fluoro-L-alanine and 2-deutero-3-fluoro-L-alanine to their D-isomers
INVENTOR(S): Reinhold, Donald F.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 5 pp. Continuation-in-part of U.S. 3,880,922.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3950411	A	19760413	US 1975-552474	19750224
US 3880922	A	19750429	US 1972-223292	19720203
FI 7600302	A	19760825	FI 1976-302	19760209
SE 7601423	A	19760825	SE 1976-1423	19760210
DK 7600559	A	19760825	DK 1976-559	19760211
NO 7600448	A	19760825	NO 1976-448	19760212
NL 7601511	A	19760826	NL 1976-1511	19760213
AU 7611178	A1	19770825	AU 1976-11178	19760217
AU 500536	B2	19790524		
CH 620194	A	19801114	CH 1976-1930	19760217
CA 1045157	A1	19781226	CA 1976-246060	19760218
GB 1488332	A	19771012	GB 1976-6655	19760219
FR 2301513	A1	19760917	FR 1976-4715	19760220
FR 2301513	B1	19790202		
ES 445381	A1	19770601	ES 1976-445381	19760220
DE 2607252	A1	19760902	DE 1976-2607252	19760223
CS 199274	P	19800731	CS 1976-1182	19760223
JP 51110513	A2	19760930	JP 1976-18580	19760224
HU 173362	P	19790428	HU 1976-ME1954	19760224

PRIORITY APPLN. INFO.: US 1972-223292 19720203
US 1975-552474 19750224

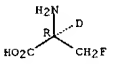
IT **35455-21-1 59189-05-8**
RL: PROC (Process)
(asymmetric conversion of)
RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



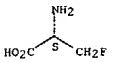
RN 59189-05-8 CAPLUS
CN L-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



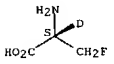
IT **35455-20-0P 35523-45-6P 59189-06-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

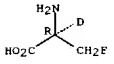


RN 59189-06-9 CAPLUS
CN L-Alanine-2-d, 3-fluoro-, benzenesulfonate (9CI) (CA INDEX NAME)

CM 1

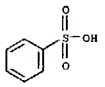
CRN 59189-05-8
CMF C3 H5 D F N O2

Absolute stereochemistry.



CM 2

CRN 98-11-3
CMF C6 H6 O3 S



AB 2-Deutero-3-fluoro-DL-alanine benzenesulfonate was resolved by crystallization
Treatment of the D-isomer with dilute NH3 gave 3-deutero-3-fluoro-D-alanine useful as a bactericide (no data).

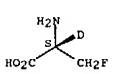
ACCESSION NUMBER: 1976:180629 CAPLUS
DOCUMENT NUMBER: 84:180629
TITLE: Resolution of 2-deutero-3-fluoro-DL-alanine salts
INVENTOR(S): Reinhold, Donald F.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2534031	A1	19760212	DE 1975-2534031	19750730
NO 7502551	A	19760203	NO 1975-2751	19750717
NO 140368	C	19790822		
NO 140368	B	19790514		
CA 1054158	A1	19790508	CA 1975-231941	19750721
AU 7583316	A1	19770127	AU 1975-83316	19750723
AU 497991	B2	19790201		
FI 7502130	A	19760201	FI 1975-2130	19750724
CH 598194	A	19780428	CH 1975-9682	19750724
BE 831760	A1	19760126	BE 1975-158335	19750725
NL 7508925	A	19760203	NL 1975-8925	19750725
SE 7508553	A	19760202	SE 1975-8553	19750728
GB 1472396	A	19770504	GB 1975-31488	19750728
FR 2280366	A1	19760227	FR 1975-23617	19750729
FR 2280366	B1	19820730		
DD 119209	C	19760412	DD 1975-187544	19750729
DK 7503458	A	19760201	DK 1975-3458	19750730
ZA 7504918	A	19770330	ZA 1975-4918	19750730
ES 439857	A1	19770616	ES 1975-439857	19750730
SU 568362	D	19770805	SU 1975-2163062	19750730
CS 191271	P	19790629	CS 1975-5338	19750730
PL 103968	P	19790731	PL 1975-182389	19750730
JP 51039626	A2	19760402	JP 1975-92656	19750731
HU 170472	P	19770628	HU 1975-ME1881	19750731

PRIORITY APPLN. INFO.: US 1974-493352 19740731

IT **35523-45-6P 59189-06-9P 59189-07-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



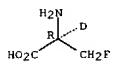
RN 59189-06-9 CAPLUS

CN L-Alanine-2-d, 3-fluoro-, benzenesulfonate (9CI) (CA INDEX NAME)

CM 1

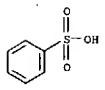
CRN 59189-05-8
CMF C3 H5 D F N O2

Absolute stereochemistry.



CM 2

CRN 98-11-3
CMF C6 H6 O3 S

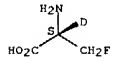


RN 59189-07-0 CAPLUS
CN D-Alanine-2-d, 3-fluoro-, benzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 35523-45-6
CMF C3 H5 D F N O2

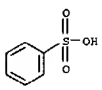
Absolute stereochemistry.



CM 2

CRN 98-11-3
CMF C6 H6 O3 S

L24 ANSWER 318 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L24 ANSWER 319 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN

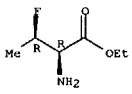
AB DL- and L-Threonine were esterified to their Me and Et esters which on treatment with SF4 in anhydrous HF gave DL- and L-Me and Et 2-amino-3-fluorobutyrates, resp. Both fluorinated esters gave on hydrolysis DL- and L-2-amino-3-fluorobutyric acid, resp.

ACCESSION NUMBER: 1976:122271 CAPLUS
DOCUMENT NUMBER: 84:122271
TITLE: The synthesis of DL- and L-2-amino-3-fluorobutyric acid
AUTHOR(S): Loy, R. S.; Hudlicky, M.
CORPORATE SOURCE: Dep. Chem., Virginia Polytech. Inst., Blacksburg, VA, USA
SOURCE: Journal of Fluorine Chemistry (1976), 7(4), 421-6
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **58960-34-2P 58960-35-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

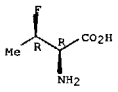
RN 58960-34-2 CAPLUS
CN Butanoic acid, 2-amino-3-fluoro-, ethyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 58960-35-3 CAPLUS
CN Butanoic acid, 2-amino-3-fluoro-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 320 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN

AB Treatment of D-PhCHMeNH2 with FCH2COCO2H gave FCH2C(:NHCHMePh)CO2H which was hydrogenated with Pd/C followed by hydrogenolysis to give the bactericidal (no data) 3-fluoro-D-alanine. Hydrogenation with deuterium gave 2-deutero-3-fluoro-D-alanine.

ACCESSION NUMBER: 1976:106074 CAPLUS
DOCUMENT NUMBER: 84:106074
TITLE: 3-Fluoro-D-alanine
INVENTOR(S): Reinhold, Donald F.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 2 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

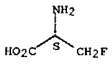
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3929576	A	19751230	US 1974-525591	19741120
NL 7300577	A	19730807	NL 1973-577	19730115
CS 178418	P	19770915	CS 1973-478	19730122
AU 7351369	A1	19740725	AU 1973-51369	19730123
CA 1001652	A1	19761214	CA 1973-161915	19730124
AT 324294	B	19750825	AT 1973-790	19730130
ES 411143	A1	19751201	ES 1973-411143	19730131
PL 84511	P	19760430	PL 1973-160498	19730131
DD 108522	C	19740920	DD 1973-168612	19730201
GB 1380382	A	19750115	GB 1973-5087	19730201
DD 114594	C	19750812	DD 1973-181401	19730201
JP 48085524	A2	19731113	JP 1973-13024	19730202
ZA 7300777	A	19741030	ZA 1973-777	19730202
SU 485592	D	19750925	SU 1973-1878868	19730202
HU 168659	P	19760628	HU 1973-ME1599	19730202
CH 585694	A	19770315	CH 1973-1489	19730202
FR 2197859	A1	19740329	FR 1973-35004	19731001

PRIORITY APPLN. INFO.: US 1972-223355 19720203

IT **35455-20-0P 35523-45-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

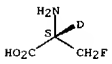
Absolute stereochemistry. Rotation (-).



RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L24 ANSWER 320 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L24 ANSWER 321 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN

AB Treatment of FCH2CHO with D-PhCHMeNH2 gave the corresponding acetaldimine which then reacted with HCN to give D-PhCHMeNHCH(CN)CH2F. Acid hydrolysis of the propionitrile followed by methylbenzyl cleavage by hydrolysis gave 3-fluoro-D-alanine useful as a bactericide (no data).

ACCESSION NUMBER: 1976:106072 CAPLUS
DOCUMENT NUMBER: 84:106072
TITLE: 3-Fluoro-D-alanine
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Austrian, 3 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

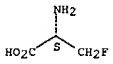
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 326096	B	19751125	AT 1973-789	19730130
AT 7300789	A	19750215		
US 3903150	A	19750902	US 1972-223340	19720203
NL 7300575	A	19730807	NL 1973-575	19730115
SE 402008	C	19780921	SE 1973-698	19730118
CA 1001650	A1	19761214	CA 1973-161903	19730124
PL 84510	P	19760430	PL 1973-160435	19730127
ES 411142	A1	19751201	ES 1973-411142	19730131
DD 108074	C	19740912	DD 1973-168609	19730201
SU 484682	D	19750915	SU 1973-1878072	19730201
JP 48085522	A2	19731113	JP 1973-13022	19730202
HU 169231	P	19761028	HU 1973-ME1600	19730202
CH 582648	A	19761215	CH 1973-1488	19730202

PRIORITY APPLN. INFO.: US 1972-223340 19720203

IT **35455-20-0P 39621-34-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

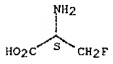
Absolute stereochemistry. Rotation (-).



RN 39621-34-6 CAPLUS
CN D-Alanine, 3-fluoro-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L24 ANSWER 321 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



● HCl

L24 ANSWER 322 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN

AB 3-Fluoro-D-alanine, prepared by treatment of D-alanine with HF-FOC F3 for 1 hr, had ED50 of 0.104-0.897 mg s. against 7 bacterial strains. Deuterration of D-alanine gave the 2-deutero-D-alanine in 95% yield which was then fluorinated in the 3 position.

ACCESSION NUMBER: 1975:497936 CAPLUS
DOCUMENT NUMBER: 83:97936
TITLE: 3-Fluoro-D-alanine, 2-deutero-3-fluoro-D-analine, or 2,3,3-trideutero-3-fluoro-D-alanine and their salts
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Austrian, 5 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

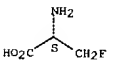
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 322524	B	19750526	AT 1971-10813	19711216
AT 332859	B	19761025	AT 1974-3124	19740416
AT 7403124	A	19760215		

PRIORITY APPLN. INFO.: AT 1971-10813 19711216

IT **35455-20-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)

RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

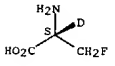
Absolute stereochemistry. Rotation (-).



IT **35523-45-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 323 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN

GI For diagram(s), see printed CA Issue.

AB The undesired property of autoantagonism exhibited by 3-fluoro-D-alanine [**35455-20-0**] type agents was completely suppressed by cycloserine derivs. I (R = H or Me, R' = H or alkyl). E.g., cycloserine [68-41-7] was treated with 2,4-pentanedione [123-54-6] to give D-4-(1-methyl-3-oxo-1-butenylamino)-3-isoxazolidinone (II) [55694-83-2]. Bactericidal agents in suitable carriers for oral administration and for injection were prepared from the combinations of these autoantagonist inhibitors e.g., II Na salt [55851-86-0] or II Ca salt [55851-87-1] with 3-fluoro-D-alanine derivs.

ACCESSION NUMBER: 1975:484873 CAPLUS
DOCUMENT NUMBER: 83:84873
TITLE: Bactericidal composition containing a 3-fluoro-D-alanine and a cycloserine
INVENTOR(S): Kahan, Frederick M.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2436959	A1	19750220	DE 1974-2436959	19740731
DE 2436959	C2	19870305		
ZA 7404366	A	19750730	ZA 1974-4366	19740708
NL 7409574	A	19750212	NL 1974-9574	19740715
NL 181407	B	19870316		
NL 181407	C	19870817		
AU 7471250	A1	19760115	AU 1974-71250	19740715
GB 1457950	A	19761208	GB 1974-32360	19740722
CA 1039191	A1	19780926	CA 1974-205968	19740730
BE 818335	A4	19750131	BE 1974-147155	19740731
FR 2240000	A2	19750307	FR 1974-27593	19740808

PRIORITY APPLN. INFO.: US 1973-387571 19730810
US 1974-478793 19740613

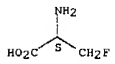
L24 ANSWER 324 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB 3-Fluoro-D-alanine (I), useful as a bactericide (no data), was prepared by
treatment of 3-fluoro-L-alanine with HBr and NaNO2 to give L-2-bromo-3-fluoropropionic acid which underwent ammonolysis with liquid NH3
or treatment with NaN3 to give the 2-azido derivative hydrogenation of which
with Pd/C gave I. Me 2-carboxy-3-fluoropropionate was prepared and resolved
to give the S-isomer which reacted with NaN3 to give Me S-2-azidocarbonyl-3-fluoropropionate which underwent decomposition to the 2-isocyanato and hydrolysis to give I.
ACCESSION NUMBER: 1975:443747 CAPLUS
DOCUMENT NUMBER: 83:43747
TITLE: 3-Fluoro-D-alanine by asymmetric rearrangement of 2-(azidocarbonyl)-3-fluoro-propionic ester or nitrile
INVENTOR(S): Reinhold, Donald F.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 4 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3880922	A	19750429	US 1972-223292	19720203
CH 586654	A	19770415	CH 1972-18918	19721227
NL 7300631	A	19730807	NL 1973-631	19730116
SE 402007	C	19780921	SE 1973-696	19730118
PL 84478	P	19760430	PL 1973-160398	19730124
CA 1001651	A1	19761214	CA 1973-161912	19730124
DD 103889	C	19740212	DD 1973-168486	19730125
AT 7300792	A	19750215	AT 1973-792	19730130
AT 326097	B	19751125		
ES 411140	A1	19760316	ES 1973-411140	19730131
CS 178419	P	19770915	CS 1973-742	19730131
SU 550976	D	19770315	SU 1973-1878069	19730201
JP 48085521	A2	19731113	JP 1973-13021	19730202
HU 170186	P	19770428	HU 1973-ME1601	19730202
US 3950411	A	19760413	US 1975-552474	19750224
ES 438617	A1	19770316	ES 1975-438617	19750616
ES 438616	A1	19770416	ES 1975-438616	19750616

PRIORITY APPLN. INFO.: US 1972-223292 19720203
IT **35455-20-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(bactericide, preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

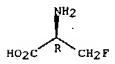
Absolute stereochemistry. Rotation (-).

L24 ANSWER 324 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **35455-21-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(epimerization of)
RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

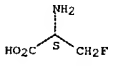


L24 ANSWER 325 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB Bactericidal (no data) 3-fluoro-D-alanine was prepared via selective asymmetric hydrolysis of N-chloroacetyl-3-fluoro-DL-alanine with Renalacylase I to give 3-fluoro-L-alanine, which crystallized out, and N-chloroacetyl-3-fluoro-D-alanine, which was hydrolyzed with 2N aqueous HCl
for 2 hr at 100°.
ACCESSION NUMBER: 1975:410859 CAPLUS
DOCUMENT NUMBER: 83:10859
TITLE: 3-Fluoro-D-alanine
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Austrian, 2 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 317123	B	19740812	AT 1973-793	19730130
NL 7300578	A	19730807	NL 1973-578	19730115
CS 171275	P	19761029	CS 1973-476	19730122
PL 84477	P	19760430	PL 1973-160434	19730127
ES 411141	A1	19751201	ES 1973-411141	19730131
DD 106164	C	19740612	DD 1973-168611	19730201
SU 484683	D	19750915	SU 1973-1878073	19730201
JP 48085789	A2	19731113	JP 1973-13025	19730202
CH 575355	A	19760514	CH 1973-1486	19730202

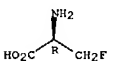
PRIORITY APPLN. INFO.: US 1972-223293 19720203
IT **35455-20-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(bactericide, preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **35455-21-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

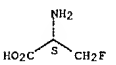


L24 ANSWER 326 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB D-FCH2CH(NH2)CO2H was prepared by treating D-PhCHMeNH2 with FCH2COCO2H, hydrogenating the D-PhCHMeN:C(CH2F)CO2H over Pd-C and debenzylating in a 2nd hydrogenation step. When the hydrogenation was carried out with deuterium, DFCH2CD(NH2)CO2H was obtained.
ACCESSION NUMBER: 1974:83648 CAPLUS
DOCUMENT NUMBER: 80:83648
TITLE: Asymmetric synthesis of 3-fluoro-D-alanine
INVENTOR(S): Reinhold, Donald F.
PATENT ASSIGNEE(S): Merck and Co., Inc.
SOURCE: Fr. Demande, 6 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2170180	A1	19730914	FR 1973-3666	19730202
FR 2170180	B1	19770422		
NL 7300577	A	19730807	NL 1973-577	19730115
CS 178418	P	19770915	CS 1973-478	19730122
AU 7351369	A1	19740725	AU 1973-51369	19730123
CA 1001652	A1	19761214	CA 1973-161915	19730124
AT 324294	B	19750825	AT 1973-790	19730130
ES 411143	A1	19751201	ES 1973-411143	19730131
PL 84511	P	19760430	PL 1973-160498	19730131
DD 108522	C	19740920	DD 1973-168612	19730201
GB 1380382	A	19750115	GB 1973-5087	19730201
DD 114594	C	19750812	DD 1973-181401	19730201
JP 48085524	A2	19731113	JP 1973-13024	19730202
ZA 7300777	A	19741030	ZA 1973-777	19730202
SU 485592	D	19750925	SU 1973-1878868	19730202
HU 168659	P	19760628	HU 1973-ME1599	19730202
CH 585694	A	19770315	CH 1973-1489	19730202
FR 2197859	A1	19740329	FR 1973-35004	19731001

PRIORITY APPLN. INFO.: US 1972-223355 19720203
IT **35455-20-0P 35523-45-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

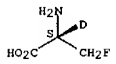
Absolute stereochemistry. Rotation (-).



RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L24 ANSWER 326 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L24 ANSWER 327 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN

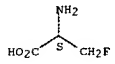
AB 3-Fluoro-D-alanine (I) and D-cycloserine, a I-autoantangonist inhibitor, had synergistic bactericidal effects, especially against Staphylococcus aureus,
Proteus morganii, Serratia species, and Escherichia coli in mice.

ACCESSION NUMBER: 1973:529095 CAPLUS
DOCUMENT NUMBER: 79:129095
TITLE: Bactericidal composition
INVENTOR(S): Kahan, Frederick M.
PATENT ASSIGNEE(S): Merck and Co., Inc.
SOURCE: Ger. Offen., 14 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2262787	A1	19730809	DE 1972-2262787	19721221
DE 2262787	C2	19820923		
NL 7300636	A	19730807	NL 1973-636	19730116
NL 177183	B	19850318		
NL 177183	C	19850816		
AU 7351368	A1	19740725	AU 1973-51368	19730123
CA 1024448	A1	19780117	CA 1973-161913	19730124
GB 1421023	A	19760114	GB 1973-4426	19730129
BE 794913	A1	19730802	BE 1973-127197	19730202
FR 2181703	A1	19731207	FR 1973-3668	19730202
ZA 7300761	A	19740925	ZA 1973-761	19730202
PRIORITY APPLN. INFO.:			US 1972-223360	19720203
			US 1972-314878	19721213

IT **35455-20-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); BIOL (Biological study)
(bactericide, cycloserine and)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L24 ANSWER 328 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN

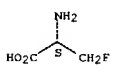
AB Bactericides 3-fluoro-D-alanine (I), and D-FCH2CD(NH2)CO2H (II), were prepared from FCH2COCO2H (III). Thus, III reacted with D-PhCHMeNH2 at 0° to give D-FCH2C(:NCHMePh)CO2H, which reacted with H or D over Pd/C to give, after hydrogenolytic cleavage of the methylbenzyl group, I or II, resp. I was also prepared by treatment of III Na salt with pig kidney D-amino acid oxidase in the presence of (NH4)2SO4 and D-proline under N at pH 8.5.

ACCESSION NUMBER: 1973:515888 CAPLUS
DOCUMENT NUMBER: 79:115888
TITLE: 3-Fluoro-D-alanine
INVENTOR(S): Reinhold, Donald F.
PATENT ASSIGNEE(S): Merck and Co., Inc.
SOURCE: Ger. Offen., 7 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2305256	A1	19730809	DE 1973-2305256	19730202
NL 7300577	A	19730807	NL 1973-577	19730115
CS 178418	P	19770915	CS 1973-478	19730122
AU 7351369	A1	19740725	AU 1973-51369	19730123
CA 1001652	A1	19761214	CA 1973-161915	19730124
AT 324294	B	19750825	AT 1973-790	19730130
ES 411143	A1	19751201	ES 1973-411143	19730131
PL 84511	P	19760430	PL 1973-160498	19730131
DD 108522	C	19740920	DD 1973-168612	19730201
GB 1380382	A	19750115	GB 1973-5087	19730201
DD 114594	C	19750812	DD 1973-181401	19730201
JP 48085524	A2	19731113	JP 1973-13024	19730202
ZA 7300777	A	19741030	ZA 1973-777	19730202
SU 485592	D	19750925	SU 1973-1878868	19730202
HU 168659	P	19760628	HU 1973-ME1599	19730202
CH 585694	A	19770315	CH 1973-1489	19730202
FR 2197859	A1	19740329	FR 1973-35004	19731001
PRIORITY APPLN. INFO.:			US 1972-223355	19720203

IT **35455-20-0P 35523-45-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

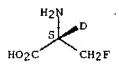
Absolute stereochemistry. Rotation (-).



RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L24 ANSWER 328 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

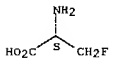


L24 ANSWER 329 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB Antibacterial 3-fluoro-D-alanine (D-I), more active than its L-isomer (L-I), was separated continuously (optionally as salt, e.g., benzenesulfonate) by supersatg. an aqueous solution of DL-I at .apprx.30°, inoculating with L-I at .apprx.25°, crystallizing L-I and inoculating the mother liquor with D-I to give crystalline D-I. The mother liquor was recycled. L-I was racemized via its acetyl derivative and recycled.
ACCESSION NUMBER: 1973:515887 CAPLUS
DOCUMENT NUMBER: 79:115887
TITLE: Separation of antibacterial 3-fluoro-D-alanine
INVENTOR(S): Reinhold, Donald F.
PATENT ASSIGNEE(S): Merck and Co., Inc.
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2305187	A1	19730809	DE 1973-2305187	19730202
HU 168658	P	19760628	HU 1972-ME1597	19720202
NL 7300576	A	19730807	NL 1973-576	19730115
CS 174867	P	19770429	CS 1973-479	19730122
AU 7351371	A1	19740725	AU 1973-51371	19730123
CA 1001656	A1	19761214	CA 1973-161902	19730124
GB 1386044	A	19750305	GB 1973-4428	19730129
AT 7300791	A	19750815	AT 1973-791	19730130
AT 329529	B	19760510		
DD 105210	C	19740412	DD 1973-168608	19730201
PL 100022	P	19780831	PL 1973-160524	19730201
FR 2170181	A1	19730914	FR 1973-3667	19730202
JP 48085523	A2	19731113	JP 1973-13023	19730202
ZA 7300760	A	19740925	ZA 1973-760	19730202
CH 591407	A	19770915	CH 1973-1490	19730202
PRIORITY APPLN. INFO.:			US 1972-223357	19720203

IT **35455-20-0P 35455-21-1P**
RL: PREP (Preparation)
(manufacture of, by resolution through crystallization)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

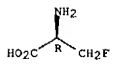
Absolute stereochemistry. Rotation (-).



RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L24 ANSWER 329 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

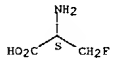


IT **42717-00-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42717-00-0 CAPLUS
CN D-Alanine, 3-fluoro-, benzenesulfonate (9CI) (CA INDEX NAME)

CM 1

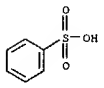
CRN 35455-20-0
CMF C3 H6 F N O2

Absolute stereochemistry. Rotation (-).



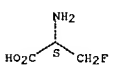
CM 2

CRN 98-11-3
CMF C6 H6 O3 S



L24 ANSWER 330 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB A highly active antibacterial agent, which is active against gram-neg. and pos. bacteria, was prepared by C-fluorination of a key component of the bacterial cell wall, D-alanine [338-69-2]. Thus, 3-fluoro-D-alanine [**35455-20-0**] at concns. of 6-100 μg/ml inhibited the growth of Escherichia coli. D-alanine at 6-100 μg/ml reversed the inhibitory effect of 3-fluoro-D-alanine at 25 μg/ml. The ED50 values of 3-fluoro-D-alanine for Streptococcus pyrogenes and Diplococcus pneumoniae in mice were 1.1 and 5 mg/kg, resp. Mice survived a single, oral dose of 2 g/kg.
ACCESSION NUMBER: 1973:474171 CAPLUS
DOCUMENT NUMBER: 79:74171
TITLE: New antibacterial agent via photofluorination of a bacterial cell wall constituent
AUTHOR(S): Kollonitsch, J.; Barash, L.; Kahan, F. M.; Kropp, H.
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Rahway, NJ, USA
SOURCE: Nature (London, United Kingdom) (1973), 243(5406), 346-7
CODEN: NATUAS; ISSN: 0028-0836
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **35455-20-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(bactericidal activity of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



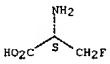
L24 ANSWER 331 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB D-FCH2CH(NH2)CO2H (D-I), D-FCH2CD(NH2)CO2H (II), and D-FCHDCD(NH2)CO2H, useful as bactericides, were prepared either by resolution of DL-I or by syntheses. Thus, DL-I was N-protected by reaction with PhCH2O2CCl, then the salt with L-tyrosine hydrazide was formed, fractionally crystallized, and cleaved by treatment with dilute HCl, and the N-protective group cleaved off by hydrogenation to give D-I. Starting materials for the synthesis of D-I were FCH:C(NHBz)CO2H, D(+)-PhCHMeNH2 and FCH2CHO or FCH2COCO2H, and others. Treatment of the intermediate D-FCH2C(:NCHMePh)CO2H with D, followed by hydrogenolysis, gave II.
ACCESSION NUMBER: 1973:72586 CAPLUS
DOCUMENT NUMBER: 78:72586
TITLE: 3-Fluoro-D-alanine and deuterio derivatives
INVENTOR(S): Kollonitsch, Janos
PATENT ASSIGNEE(S): Merck and Co., Inc.
SOURCE: Ger. Offen., 24 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2229245	A	19721221	DE 1972-2229245	19720615
NL 7207606	A	19721220	NL 1972-7606	19720605
FI 57745	B	19800630	FI 1972-1587	19720606
FI 57745	C	19801010		
CS 189580	P	19790430	CS 1972-4076	19720612
DD 106364	C	19740612	DD 1972-163666	19720613
DD 108976	C	19741012	DD 1972-175715	19720613
GB 1389858	A	19750409	GB 1972-27621	19720613
GB 1389859	A	19750409	GB 1974-13200	19720613
CA 994800	A1	19760810	CA 1972-144614	19720613
AT 7205115	A	19760415	AT 1972-5115	19720614
AT 333717	B	19761210		
FR 2142474	A5	19730126	FR 1972-21616	19720615
PL 90080	P	19761231	PL 1972-156081	19720615
CH 584186	A	19770131	CH 1972-8945	19720615
ES 403932	A1	19751116	ES 1972-403932	19720616
CA 968368	A2	19750527	CA 1974-205439	19740723
CA 994360	A2	19760803	CA 1974-210939	19741008
ES 431083	A1	19770116	ES 1974-431083	19741016
AT 7408827	A	19760315	AT 1974-8827	19741104
AT 333246	B	19761110		
AT 7502890	A	19760815	AT 1975-2890	19750416
AT 335992	B	19770412		
PRIORITY APPLN. INFO.:			US 1971-154695	19710618
			US 1972-223354	19720203
			US 1970-60645	19700803
			CA 1971-118803	19710721
			CA 1972-144614	19720613
			AT 1972-5115	19720614

IT **35455-20-0P 35523-45-6P 39621-34-6P 39621-36-8P 39741-57-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

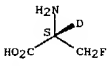
L24 ANSWER 331 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



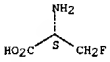
RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 39621-34-6 CAPLUS
CN D-Alanine, 3-fluoro-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



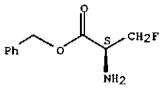
● HCl

RN 39621-36-8 CAPLUS
CN D-Alanine, 3-fluoro-, phenylmethyl ester, [R-(R*,R*)]-2,3-bis(benzoyloxy)butanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 46344-20-1
CMF C10 H12 F N O2

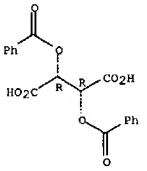
Absolute stereochemistry.



CM 2

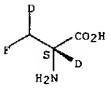
L24 ANSWER 331 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CRN 2743-38-6
CMF C18 H14 O8

Absolute stereochemistry.



RN 39741-57-6 CAPLUS
CN D-Alanine-2,3-d2, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 332 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB Fluoroxytrifluoromethane [373-91-1] is used in uv light to convert benzene
to fluorobenzene [462-06-6], toluene to a mixture of 2-fluorotoluene and PhCH2F, cyclohexane to fluorocyclohexane, EtNH2 to FCH2CH2NH2, HCF2CH2NH2,
or CF3CH2NH2, polycaprolactam (I) [25038-54-4], polyethylene [9002-88-4], polystyrene [9003-53-6], and a siloxane to fluorinated polymers containing
17.3, 3.1, 2.45, and 34% F, resp., AcOH to FCH2CO2H, 4-(PhCH2CH2)C6H4CMe2NH2 to 4-(PhCF2CF2)C6H4CMe2NH2, etc.
Fluoroxypentafluorosulfur [15179-32-5] and fluoroxyperfluoroethane [3848-94-0] are used to prepare PhF from benzene and fluorocyclohexane from
cyclohexane, resp. Thus, 1.13 g I in 40 ml HF is treated with 3.6 g CF3OF
under uv light at -78.deg. to prepare fluorinated I containing 17.3% F.

ACCESSION NUMBER:	1972:154488 CAPLUS
DOCUMENT NUMBER:	76:154488
TITLE:	Fluorination of organic compounds in the presence of a free radical-producing initiator
INVENTOR(S):	Kollonitsch, Janos
PATENT ASSIGNEE(S):	Merck and Co., Inc.
SOURCE:	Ger. Offen., 40 pp. CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	6

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2136008	A	19720210	DE 1971-2136008	19710719
DE 2136008	B2	19760212		
DE 2136008	C3	19761014		
NL 7109946	A	19720207	NL 1971-9946	19710719
NL 173388	B	19830816		
NL 173388	C	19840116		
AU 7131463	A1	19730125	AU 1971-31463	19710720
CA 967982	A1	19750520	CA 1971-118803	19710721
IT 988052	A	19750410	IT 1971-51835	19710722
GB 1353519	A	19740522	GB 1971-34887	19710726
FR 2101198	A5	19720331	FR 1971-28394	19710803
FR 2101198	B1	19750801		
FR 2103901	A5	19720414	FR 1971-28393	19710803
ZA 7105185	A	19730328	ZA 1971-5185	19710803
HU 163751	P	19731027	HU 1971-ME1404	19710803
HU 166452	P	19750328	HU 1971-ME1550	19710803
CH 575354	A	19760514	CH 1971-11408	19710803
JP 55044048	B4	19801110	JP 1971-58028	19710803
FR 2142474	A5	19730126	FR 1972-21616	19720615
CA 968368	A2	19750527	CA 1974-205439	19740723
CA 994360	A2	19760803	CA 1974-210939	19741008
AT 7408827	A	19760315	AT 1974-8827	19741104
AT 333246	B	19761110		

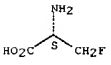
PRIORITY APPLN. INFO.:	US 1970-60645	19700803
	US 1971-154695	19710618
	CA 1971-118803	19710721
	US 1972-223354	19720203

L24 ANSWER 332 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

	CA 1972-144614	19720613
	AT 1972-5115	19720614

IT **35455-20-0P**
RL: PREP (Preparation)
(preparation of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



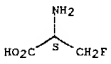
L24 ANSWER 333 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB The title compds. and 3-fluoro-D-alanine-2-2H were prepared by reaction of
the alanines with F3COF in HF in the presence of uv light and used as antibacterial substances. Thus, F3COF was passed into (-)-D-alanine in liquid HF with uv irradiation to give 41% 3-fluoro-D-alanine.
ACCESSION NUMBER: 1972:100053 CAPLUS
DOCUMENT NUMBER: 76:100053
TITLE: Antibacterial 3-fluoro-L- and -D-alanine
INVENTOR(S): Kollonitsch, Janos; Kahan, Frederick M.
PATENT ASSIGNEE(S): Merck and Co., Inc.
SOURCE: Ger. Offen., 17 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2136067	A	19720210	DE 1971-2136067	19710719
DE 2136067	B2	19800117		
DE 2136067	C3	19800911		
NL 7109947	A	19720207	NL 1971-9947	19710719
NL 174248	B	19831216		
NL 174248	C	19840516		
AU 7131464	A1	19730125	AU 1971-31464	19710720
CA 956646	A1	19741022	CA 1971-118804	19710721
GB 1367674	A	19740918	GB 1971-34886	19710726
BE 770888	A1	19720203	BE 1971-106700	19710803
FR 2101198	A5	19720331	FR 1971-28394	19710803
FR 2101198	B1	19750801		
FR 2103901	A5	19720414	FR 1971-28393	19710803
ZA 7105185	A	19730328	ZA 1971-5185	19710803
HU 166452	P	19750328	HU 1971-ME1550	19710803
IL 37429	A1	19750522	IL 1971-37429	19710803
CH 563961	A	19750715	CH 1971-11407	19710803
JP 56005217	B4	19810204	JP 1971-58027	19710803
CA 968368	A2	19750527	CA 1974-205439	19740723

PRIORITY APPLN. INFO.: US 1970-60645 19700803
US 1971-149814 19710603
US 1971-154695 19710618
CA 1971-118803 19710721

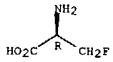
IT **35455-20-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); IMF (Industrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture and antibacterial activity of)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



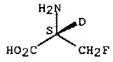
L24 ANSWER 333 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
IT **35455-21-1P 35523-45-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



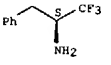
RN 35523-45-6 CAPLUS
CN D-Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 334 OF 334 CAPLUS COPYRIGHT 2004 ACS on STN
AB The area of the enzyme which complexes the benzene ring of L-phenylalanine
represents the primary site of recognition and one of the two major binding loci. This region is best described as a hydrophobic pocket with a stringent steric requirement for the phenyl ring of the substrate; substituents on the benzene ring which are larger than H invariably lead to a loss of substrate activity and binding energy. The other major binding locus is that which complexes the protonated amino group of L-phenylalanine and related analogs, and is probably best represented as an anionic group of the enzyme. This region also has rigid steric requirements for binding and substrate activity and is intolerant of substituents on the amine which are larger than H. The stereospecificity of the enzyme is exact with regard to substrate and binding properties and
appears to be governed by steric constraints in the region of the binding site which is occupied by the α hydrogen of L-phenylalanine. The presence of the α-carboxyl group is not necessary for optimal binding.
ACCESSION NUMBER: 1972:22491 CAPLUS
DOCUMENT NUMBER: 76:22491
TITLE: Phenylalanyl transfer ribonucleic acid synthetase from
Escherichia coli. Analysis of the phenylalanine binding site
AUTHOR(S): Santi, Daniel V.; Danenberg, Peter V.
CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA, USA
SOURCE: Biochemistry (1971), 10(25), 4813-20
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **35373-60-5**
RL: BIOL (Biological study)
(phenylalanyl-transfer ribonucleate synthetase inhibition by, kinetics of)
RN 35373-60-5 CAPLUS
CN Benzeneethanamine, α-(trifluoromethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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 NEWS  3  JAN 27   Source of Registration (SR) information in REGISTRY updated
                   and searchable
 NEWS  4  JAN 27   A new search aid, the Company Name Thesaurus, available in
                   CA/CAplus
 NEWS  5  FEB 05   German (DE) application and patent publication number format
                   changes
 NEWS  6  MAR 03   MEDLINE and LMEDLINE reloaded
 NEWS  7  MAR 03   MEDLINE file segment of TOXCENTER reloaded
 NEWS  8  MAR 03   FRANCEPAT now available on STN
 NEWS  9  MAR 29   Pharmaceutical Substances (PS) now available on STN
 NEWS 10  MAR 29   WPIFV now available on STN
 NEWS 11  MAR 29   No connect hour charges in WPIFV until May 1, 2004
 NEWS 12  MAR 29   New monthly current-awareness alert (SDI) frequency in RAPRA
 NEWS 13  APR 26   PROMT: New display field available
 NEWS 14  APR 26   IFIPAT/IFIUDB/IFICDB: New super search and display field
                   available
 NEWS 15  APR 26   LITALERT now available on STN
 NEWS 16  APR 27   NLDB: New search and display fields available

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               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
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 NEWS INTER    General Internet Information
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 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION

Page 1
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DICTIONARY FILE UPDATES: 4 MAY 2004 HIGHEST RN 679784-15-7

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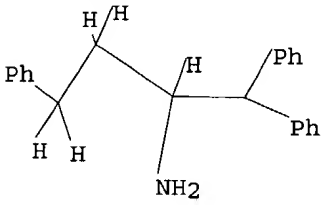
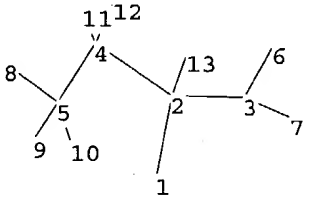
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\09857465.str



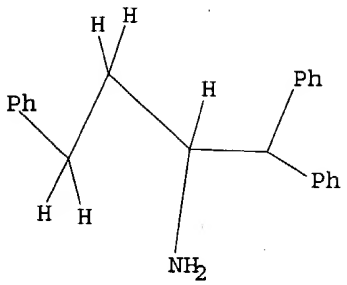


chain nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
1-2 2-3 2-4 2-13 3-6 3-7 4-5 4-11 4-12 5-8 5-9 5-10
exact/norm bonds :
1-2
exact bonds :
2-3 2-4 2-13 3-6 3-7 4-5 4-11 4-12 5-8 5-9 5-10

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS

L1 STRUCTURE UPLOADED

=> d query
L1 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 18:11:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     36 TO ITERATE

100.0% PROCESSED      36 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:          360 TO     1080
PROJECTED ANSWERS:               0 TO        0

L2             0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 18:12:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    970 TO ITERATE

100.0% PROCESSED     970 ITERATIONS                               0 ANSWERS
SEARCH TIME: 00.00.01

L3             0 SEA SSS FUL L1

=> logoff y
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              155.42     155.63

STN INTERNATIONAL LOGOFF AT 18:12:09 ON 05 MAY 2004
```